# **Open-Source CFD Course**

A course at Chalmers University of Technology Taught by Håkan Nilsson Based on OpenFOAM v2112

Presenter:

Saeed Salehi



UNIVERSITY OF TECHNOLOGY

Division of Fluid Dynamics Department of Mechanics and Maritime Sciences Chalmers University of Technology

September 2022

• The main steps are similar for both SIMPLE and PISO pressure correction algorithms.



- The main steps are similar for both SIMPLE and PISO pressure correction algorithms.
- SIMPLE algorithm, originally developed for steady physics, does not care about the fact the H(u) operator was constructed using a velocity that did not fulfill continuity.
- SIMPLE goes all the way back to the beginning of the loop and proceeds in time.



- The main steps are similar for both SIMPLE and PISO pressure correction algorithms.
- SIMPLE algorithm, originally developed for steady physics, does not care about the fact the H(u) operator was constructed using a velocity that did not fulfill continuity.
- SIMPLE goes all the way back to the beginning of the loop and proceeds in time (iteration).
- PISO was developed for unsteady physics and is intended to provide time accurate results.
- $\bullet$  PISO goes back to correction of  $\mathbf{H}(\mathbf{u})$  and performs the momentum corrector step again. Then it proceeds in time.



- The main steps are similar for both SIMPLE and PISO pressure correction algorithms.
- SIMPLE algorithm, originally developed for steady physics, does not care about the fact the H(u) operator was constructed using a velocity that did not fulfill continuity.
- SIMPLE goes all the way back to the beginning of the loop and proceeds in time (iteration).
- PISO was developed for unsteady physics and is intended to provide time accurate results.
- $\bullet$  PISO goes back to correction of  $\mathbf{H}(\mathbf{u})$  and performs the momentum corrector step again. Then it proceeds in time.





- The main steps are similar for both SIMPLE and PISO pressure correction algorithms.
- SIMPLE algorithm, originally developed for steady physics, does not care about the fact the H(u) operator was constructed using a velocity that did not fulfill continuity.
- SIMPLE goes all the way back to the beginning of the loop and proceeds in time (iteration).
- PISO was developed for unsteady physics and is intended to provide time accurate results.
- $\bullet$  PISO goes back to correction of  $\mathbf{H}(\mathbf{u})$  and performs the momentum corrector step again. Then it proceeds in time.



- What is the drawback with the PISO algorithm for unsteady problems?
- The momentum predictor is only solved once at each time step. The linearized momentum equation uses fluxes and pressure gradient from the previous time-step. This assumption is only acceptable for very small time-steps ( $Co_{max} < 1$ ). Under-relaxation cannot be used.

- PIMPLE algorithm merges PISO (inner corrector) and SIMPLE (outer corrector) loops.
- The main idea behind the PIMPLE loop is to seek a fully converged steady-state solution with under-relaxation in each time step and proceed in time.
- PIMPLE works for  $Co_{max} >> 1$ .
- If only one outer correction loop with multiple inner loops are performed, the PIMPLE loop resembles PISO.
- Performing one inner corrector with multiple outer loops makes the procedure similar to the SIMPLE algorithm (in each time step).
- Under-relaxations can be used to have a smooth convergence in each time step.



- PIMPLE algorithm is widely used in OpenFOAM. In fact, 59 solvers out of total of 108 OpenFOAM solvers employ this pressure correction algorithm, such as: pimpleFoam, buoyantPimpleFoam, rhoPimpleFoam, sonicFoam, fireFoam, reactingFoam, sprayFoam, engineFoam, interFoam, twoPhaseEulerFoam, compressibleInterIsoFoam, cavitatingFoam, interPhaseChangeFoam
- grep -irl "while (pimple.loop())" \$FOAM\_SOLVERS | wc -1
- pimpleFoam is a more sophisticated unsteady solver compared to icoFoam and enables several additional functionalities, such as
  - $\checkmark\,$  outer correction, inner correction, and non-orthogonal correction loops
  - ✓ Mesh motion
  - ✓ Adjustable time step (based on Courant number)
  - ✓ CorrectPhi
  - ✓ Turbulence modeling
  - ✓ Multiple Reference Frame (MRF)
  - ✓ fvOptions (such as porosity)
  - ✓ Under-relaxations
  - ✓ Residual control
- pimpleFoam provides a high level of flexibility using different switches and parameters.
- All switches and parameters can be set inside the PIMPLE dictionary of fvSolution.

#### PIMPLE switches and parameters

Parameter	Туре	Default	Description
nOuterCorrectors	Integer	1	Maximum number of outer correction loops
nCorrectors	Integer	1	Maximum number of inner (PISO) correction loops
nNonOrthogonalCorrectors	Integer	0	Number of non-orthogonal correction loops
momentumPredictor	Boolean	true	Indicates whether to solve for momentum
transonic	Boolean	false	Indicates whether to use transonic algorithm (compressible solvers)
consistent	Boolean	false	Indicates whether to use "consistent" approach (SIMPLEC)
frozenFlow	Boolean	false	Indicates whether the flow system of equations should not be evolved
turbOnFinalIterOnly	Boolean	true	Indicates whether to only solve turbulence on final outer loop
finalOnLastPimpleIterOnly	Boolean	false	Indicates whether the final solver is used only on the final PIMPLE loop
ddtCorr	Boolean	true	Indicates whether the ddtCorr should be applied
correctPhi	Boolean	Dynamic mesh?	Perform flux correction functions to ensure continuity before solving momentum equation.
checkMeshCourantNo	Boolean	false	Calculate Courant number of the mesh motion
moveMeshOuterCorrectors	Boolean	false	Indicates whether to perform dynamic mesh calculations in each outer loop
solveFlow	Boolean	true	Indicates whether to solve the flow (only in sprayFoam)
SIMPLErho	Boolean	false	indicate whether to update density in SIMPLE rather than PISO (In a few solvers e.g. rhoPimpleFoam)

Flowchart of the pimpleFoam solver (some details are omitted in this flowchart, e.g., correctPhi, fvOptions, MRF, etc.)













- run function of class Time returns a boolean about whether the simulation should be continued or not. It also invokes function objects.
- Can you spot the small difference between code and flowchart? run function

```
...
if (timeIndex_ == startTimeIndex_)
{
    addProfiling(functionObjects, "functionObjects.
    start()");
    functionObjects_start();
}
else
{
    addProfiling(functionObjects, "functionObjects.
    execute()");
    functionObjects_.execute();
}
...
```





#### 

Function object, Co.,  $\Delta t$ , update time



- Increment time with "++" overloaded operator
- ++runTime or runTime++?
- Both have the same effect. However, in C++ pre-increment (++1) first increases i and then return the value but post-increment (i++) first return the value and then increase it.
- The performance of overloaded operator++ could be significantly affected since post-increment needs the creation of the temporary object.
- Form OpenFOAM-v1812 the runTime increment operator switched to pre-increment (only in ESI version).

```
Foam::Time& Foam::Time::operator++()
```

```
...
setTime(value() + deltaT_, timeIndex_ + 1);
...
```







Yes

End

End time

"==" operator



End time? Yes

End

mesh motion

No

final oute:

Outer correction loop

iter only?

Final

outer?



Inner correction loop

End time? Yes

Continue

Solve turbulence

equations and update

Reynolds stress tensor

End

 $\nabla\cdot\left(\left(a_{P}^{\mathbf{u}}\right)^{-1}\nabla p\right)=\nabla\cdot\left(\left(a_{P}^{\mathbf{u}}\right)^{-1}\mathbf{H}(\mathbf{u})\right)$ 

- The appropriate solver is read from fvSolution based on p.select(pimple.finalInnerIter()) that returns a word type which is either p or pFinal.
- In each loop the explicit non-orthogonal correction term is updated. In other words, the non-orthogonal correction loop only updates the left-hand side of pEqn, while in the pressure corrector loop both sides are updated.
- In the final non-orthogonal correction loop, the conservative face fluxes are calculated.

Outer correction loop



No

End time? Yes

End

```
/ 
    if (phi.mesh().moving())
        {
            phi -= fvc::meshPhi(U);
        }
}
```



# Under relaxation factors

- Under-relaxations are required to improve the stability of computations by decreasing the change of variables between iterations.
- They should be chosen low enough to ensure stability but high enough to have a fast convergence.
- In OpenFOAM, the numerical solution is *relaxed* in two different ways, i.e., fields and equations.

1	relaxationFactors {					
	-	fie	lds			
		{				
			р	0.6;		
		}				
		equ	ations			
		{				
			"(U k omega)"	0.7; //table ((0 0.4) (0.5 0.7));		
			"(U k omega)Final"	1.0;		
		ł				
-	}					

An exmaple of relaxationFactors dictionary in the fvSolution

• For instance, in PIMPLE loop, UEqn and p are relaxed using UEqn.relax() and p.relax().

- UEqn is a fvVectorMatrix which represents an *equation*. UEqn.relax() calls the relax() function defined in fvMatrix class.
- p is a volScalarField which represents a *field*. p.relax() calls the relax() function defined in GeometricField class.
- Note that UEqn equation is first relaxed and then solved, while a solution for p is first obtained and then the field is relaxed.
- Relaxing equations are also known as implicit relaxation while applying under-relaxation factor on a field is an explicit relaxation.

5 tmp<fvVectorMatrix> tUEqn 6 ( 7 fvm::ddt(U) + fvm::div(phi, U) 8 + MRF.DDt(U) 9 + turbulence->divDevReff(U) 10 11 fvOptions(U) 12 ): fvVectorMatrix& UEan = tUEan.ref(); 13 14 UEgn.relax(): 15 16 17 fvOptions.constrain(UEqn); 18 19 if (pimple.momentumPredictor()) ł 20 21 solve(UEqn == -fvc::grad(p)); 22 23 fvOptions.correct(U); 24 }

```
38
   // Non-orthogonal pressure corrector loop
   while (pimple.correctNonOrthogonal())
39
40
   £
41
       fvScalarMatrix pEgn
42
43
           fvm::laplacian(rAtU(), p) == fvc::div(phiHbyA)
44
        ):
45
       pEqn.setReference(pRefCell, pRefValue);
46
47
48
       pEqn.solve(mesh.solver(p.select(pimple.
           finalInnerIter()))):
49
50
       if (pimple.finalNonOrthogonalIter())
51
52
           phi = phiHbyA - pEqn.flux();
53
54
   7
55
56
   #include "continuityErrs.H"
57
   // Explicitly relax pressure for momentum corrector
58
59
   p.relax();
```

UEqn.H

pEqn.H

#### Implicit relaxation, theory

- Implicit relaxation method is also known as Patankar's Under-relaxation.
- It is shown in the linear algebra that increasing diagonal dominance of a linear system enhances the stability of the iterative linear solver.
- For example, the Jacobi and Gauss-Seidel methods only converge when the matrix is strictly diagonally dominant.
- ${\ensuremath{\,\circ}}$  Consider the following discretized equation for the general variable  $\phi$

$$a_P \phi_P^n + \sum_N a_N \phi_N^n = \mathbf{r}$$

• The diagonal dominance of this linear system could be improved by adding artificial terms to both sides of equation

$$a_P \phi_P^n + \frac{1-\alpha}{\alpha} a_P \phi_P^n + \sum_N a_N \phi_N^n = \mathbf{r} + \frac{1-\alpha}{\alpha} a_P \phi_P^{n-1}$$
$$\frac{a_P}{\alpha} \phi_P^n + \sum_N a_N \phi_N^n = \mathbf{r} + \left(\frac{a_P}{\alpha} - a_P\right) \phi_P^{n-1}$$

 $\phi_P^{n-1}$ : value of  $\phi$  from the previous iteration  $\alpha$ : under-relaxation factor

 If the linear system reaches an adequate steady-state convergence (i.e., φ<sub>P</sub><sup>n-1</sup> ≈ φ<sub>P</sub><sup>n</sup>), the artificial terms cancel out and the linear system will be equivalent to the original one.

#### Implicit relaxation, implementation

relax() function in fvMatrix class

```
1239
    template<class Type>
1240
    void Foam::fvMatrix<Tvpe>::relax()
    ſ
1241
         word name = psi_.select
1242
1243
             psi_.mesh().data::template getOrDefault<bool>
1244
             ("finalIteration", false)
1245
         ):
1246
1247
         if
            (psi_.mesh().relaxEquation(name))
1248
         Ł
1249
             relax(psi_.mesh().equationRelaxationFactor(name));
1250
         }
1251
1252 }
```

- The correct name is first constructed based on the outer correction state (e.g., U or UFinal).
- relax() reads the value of under-relaxation from fvSolution and then calls the relax(const scalar alpha) (with argument) function.

#### Implicit relaxation, implementation

$$\frac{a_P}{\alpha}\phi_P^n + \sum_N a_N\phi_N^n = \mathbf{r} + \left(\frac{a_P}{\alpha} - a_P\right)\phi_P^{n-1}$$

- relax(const scalar alpha) function first store the current diagonal coefficients (D0).
- Regardless of *α* value the matrix diagonal equality/dominance is ensured.
- The diagonal coefficients are replaced by the maximum value of absolute diagonal coefficients and sum of absolute off-diagonals. This step is carried out regardless of α value.
- The matrix is relaxed by dividing diagonal members by  $\alpha$ .
- The contribution of relaxation is added to the source term. It can be easily shown that with the current implementation, any manipulation can be done to D as long as its corresponding contribution is added to the source term.

relax(const scalar alpha) in fvMatrix class

```
. . .
```

```
Field<Type>& S = source();
scalarField& D = diag();
```

```
// Store the current unrelaxed diagonal for use in
    updating the source
scalarField DO(D);
```

```
// Calculate the sum-mag off-diagonal from the
      interior faces
scalarField sumOff(D.size(), Zero);
sumMagOffDiag(sumOff):
// Ensure the matrix is diagonally dominant...
// Assumes that the central coefficient is positive
       and ensures it is
forAll(D, celli)
ſ
   D[celli] = max(mag(D[celli]), sumOff[celli]);
3
// ... then relax
D /= alpha;
// Finally add the relaxation contribution to the
      source.
S += (D - D0)*psi .primitiveField();
```

#### Implicit relaxation, implementation

- It is seen that relaxing an equation manipulates the source term and makes the equation more explicit.
- More iterations (outer corrections) should be performed to make sure that the convergence is achieved. The under-relaxation should be used only if they are needed.
- Regardless of  $\alpha$  value, implicit relaxation guarantees matrix diagonal equality/dominance.
- Therefore, it is common to have relaxationFactors dictionary as

An exmaple of relaxationFactors dictionary in the fvSolution

```
relaxationFactors
{
    equations
    {
        ".*" 1;
    }
}
```

## Explicit relaxation

- The explicit relaxation is applied on the fields (e.g., p.relax()).
- In each iteration, after obtaining a new solution, the field is relaxed using the value from previous iteration:

$$\phi_{\text{relaxed}}^{n} = \phi^{n-1} + \alpha \left( \phi^{n} - \phi^{n-1} \right)$$

• Here again, the correct name is first constructed based on the outer correction state (e.g., p or pFinal).

• The value of under-relaxation is read and the relax(const scalar alpha) function is subsequently called. relax() function in GeometricField class

```
1110 void Foam::GeometricField<Type, PatchField, GeoMesh>::relax()
11111 {
1112
         word name = this->name();
1113
         if
1114
          (
1115
              this->mesh().data::template getOrDefault<bool>
1116
1117
                  "finalIteration".
1118
                  false
1119
              )
1120
1121
          )
1122
          ſ
              name += "Final";
1123
         }
1124
1125
1126
          if (this->mesh().relaxField(name))
1127
          ſ
              relax(this->mesh().fieldRelaxationFactor(name));
1128
         3
1129
1130 }
```

#### Explicit relaxation

relax(const scalar alpha) function in GeometricField class

```
971 void Foam::GeometricField<Type, PatchField, GeoMesh>::relax(const scalar alpha)
972 {
973 DebugInFunction
974 << "Relaxing" << nl << this->info() << " by " << alpha << endl;
975
976 operator==(prevIter() + alpha*(*this - prevIter()));
977 }</pre>
```

$$\phi_{\text{relaxed}}^{n} = \phi^{n-1} + \alpha \left( \phi^{n} - \phi^{n-1} \right)$$

- The value from the previous iteration is called using prevIter().
- What exactly does the previous iteration mean?
- In PIMPLE different iterations/loops exists (Time step, outer correction, inner correction, non-orthogonal correction, linear solver iteration).
- prevIter() returns the value of fieldPrevIterPtr\_ pointer. i.e, return \*fieldPrevIterPtr\_;.
- The pointer itself is set inside storePrevIter() function of the same class. Therefore, one should look for the place that storePrevIter() is called inside the solver.

#### Explicit relaxation

- The loop() function is called on the pimple object at the beginning of each PIMPLE outer correction loop, while (pimple.loop()).
- In the loop() function, the storePrevIterFields() from solutionControl is executed:

storePrevIterFields() function in solutionControl

```
void Foam::solutionControl::storePrevIterFields() const
160
   ſ
161
   11
        storePrevIter<label>():
162
163
       storePrevIter<scalar>():
       storePrevIter<vector>():
164
       storePrevIter<sphericalTensor>();
165
       storePrevIter<symmTensor>();
166
       storePrevIter<tensor>():
167
168 }
```

- storePrevIterFields calls the storePrevIter.
- Therefore, the explicit relaxation in PIMPLE loop uses contribution from previous outer corrector loop.
- $\bullet\,$  Unlike implicit relaxations of equations, setting explicit relaxation of fields to  $\alpha=1$  does not have any effects.