Phase-field Solver for Eutectic Transformation

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Chapter 1

Code-guide for solver eutectic

The solver has been successfully tested using OpenFOAM v6.

1.1 Compiling the solver

· Following commands should create the executable of the solver

cd \$FOAM_RUN/PhaseFieldSolverEutectic/eutectic

wclean

wmake

• The solver can be run by following the instructions in userGuide.

1.2 Further details

The implementation, client and header files of the solver have been written following OpenFOAM conventions. These are explained next with flow charts generated from the source code using Doxygen. It must be noted that the solver is based on laplacianFoam solver within OpenFOAM. Hence, it may be helpful for the user to become familiar with OpenFOAM Programmer's Guide and laplacianFoam beforehand.

Chapter 2

File Index

2.1 File List

Here is a list of all files with brief descriptions:

PhaseFieldSolverEutectic/eutectic/createFields.H	5
PhaseFieldSolverEutectic/createTol.H	8
PhaseFieldSolverEutectic/eutectic/eutectic.C	ç
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PhaseFieldSolverEutectic/readTransportProperties.H	15
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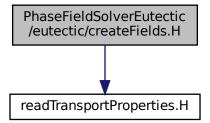
File Index

Chapter 3

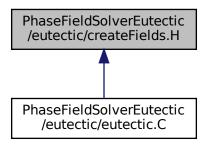
File Documentation

3.1 PhaseFieldSolverEutectic/eutectic/createFields.H File Reference

#include "readTransportProperties.H"
Include dependency graph for createFields.H:



This graph shows which files directly or indirectly include this file:



Functions

• volScalarField phi_alpha (IOobject::MUST_READ, IOobject::MUST_READ, IOobject::AUTO_WRITE), mesh)

Creating phase-fields with the option to write.

- volScalarField phi_beta (IOobject("phi_beta", runTime.timeName(), mesh, IOobject::MUST_READ, IOobject::AUTO_WRITE), mesh)
- volScalarField phi_liq (IOobject("phi_liq", runTime.timeName(), mesh, IOobject::MUST_READ, IOobject::
 AUTO WRITE), mesh)
- volScalarField T (IOobject("T", runTime.timeName(), mesh, IOobject::MUST_READ, IOobject::AUTO_← WRITE), mesh)

Creating temperature field with the option to write.

• volScalarField mu (IOobject("mu", runTime.timeName(), mesh, IOobject::MUST_READ, IOobject::AUTO_← WRITE), mesh)

Creating chemical potential field with the option to write.

3.1.1 Function Documentation

3.1.1.1 phi alpha()

Creating phase-fields with the option to write.

3.1.1.2 phi_beta()

3.1.1.3 phi_liq()

3.1.1.4 T()

Creating temperature field with the option to write.

Referenced by main().

Here is the caller graph for this function:



3.1.1.5 mu()

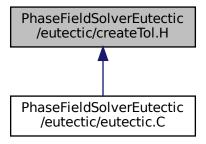
Creating chemical potential field with the option to write.

Referenced by main().



3.2 PhaseFieldSolverEutectic/eutectic/createTol.H File Reference

This graph shows which files directly or indirectly include this file:



Functions

• scalar Tol (readScalar(get_Tol_from_this.lookup("Tol")))

Initial tolerance "Tol" within subDict "Tol_is_defined_here" in fvSolution.

Variables

• const dictionary & get_Tol_from_this = mesh.solutionDict().subDict("Tol_is_defined_here")

3.2.1 Function Documentation

3.2.1.1 Tol()

Initial tolerance "Tol" within subDict "Tol_is_defined_here" in fvSolution.

3.2.2 Variable Documentation

3.2.2.1 get_Tol_from_this

```
const dictionary& get_Tol_from_this = mesh.solutionDict().subDict("Tol_is_defined_here")
```

Definition at line 1 of file createTol.H.

3.3 PhaseFieldSolverEutectic/eutectic/eutectic.C File Reference

```
#include "fvCFD.H"
#include "fvOptions.H"
#include "simpleControl.H"
#include "Random.H"
#include "setRootCase.H"
#include "createTime.H"
#include "createMesh.H"
#include "createFields.H"
#include "createTol.H"
#include "phi_abl_antiT.H"
Include dependency graph for eutectic.C:
```



Functions

• int main (int argc, char *argv[])

3.3.1 Function Documentation

3.3.1.1 main()

```
int main (
          int argc,
          char * argv[] )
```

The imposed temperature field as a function of thermal gradient in the x direction, G

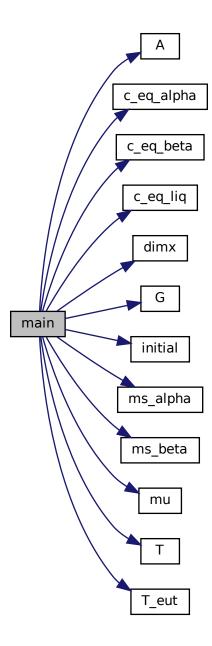
Initial tolerance to check convergence

Solving the phase-field and chemical potential equations

Writing the results according to keywords in controlDict

Definition at line 39 of file eutectic.C.

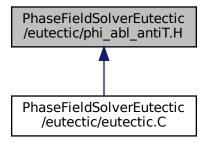
 $References\ A(),\ c_eq_alpha(),\ c_eq_beta(),\ c_eq_liq(),\ dimx(),\ G(),\ initial(),\ ms_alpha(),\ ms_beta(),\ mu(),\ T(),\ and\ T_eut().$



3.4 PhaseFieldSolverEutectic/eutectic/info.md File Reference

3.5 PhaseFieldSolverEutectic/eutectic/phi_abl_antiT.H File Reference

This graph shows which files directly or indirectly include this file:



Functions

- fvScalarMatrix phi_alphaEqn (tau *epsilon *dimt *fvm::ddt(phi_alpha) v *grad_alpha.component(vector ← ::X)==(-2.0/3.0) *(-2.0 *gamma *epsilon *dimx *dimx *fvm::laplacian(phi_alpha)+9.0 *gamma/epsilon *2.↔ 0 *(phi alpha) *(1.0-phi alpha) *(1.0-2.0 *phi alpha)+(-1.0/4.0 *(mu - B alpha) *(mu - B alpha)/A+D ← alpha) *0.25 *15 *(3.0 *phi alpha *phi alpha *phi alpha *phi alpha -4.0 *phi alpha *phi alpha *phi alpha - phi alpha *phi alpha+2.0 *phi alpha -(phi beta - phi liq) *(phi beta - phi liq) *(2.0 *phi alpha - 3.0 *phi alpha *phi alpha))+(-1.0/4.0 *(mu - B beta) *(mu - B beta)/A+D beta) *-0.5 *15 *((phi beta *phi beta - phi_beta *phi_beta *phi_beta) *(phi_alpha - phi_liq))+(-1.0/4.0 *(mu - B_liq) *(mu - B_liq)/A+D_liq) *-0.5 *15 *((phi liq *phi liq *phi liq *phi liq *phi liq *phi liq) *(phi alpha - phi beta)))+(1.0/3.0) *(-2.0 *gamma *epsilon *dimx *dimx *fvc::laplacian(phi liq)+9.0 *gamma/epsilon *2.0 *(phi liq) *(1.0-phi liq) *(1.0-2.← 0 *phi_liq)+(-1.0/4.0 *(mu - B_alpha) *(mu - B_alpha)/A+D_alpha) *-0.5 *15 *((phi_alpha *phi_alpha phi_alpha *phi_alpha *phi_alpha) *(phi_liq - phi_beta))+(-1.0/4.0 *(mu - B_beta) *(mu - B_beta)/A+D_beta) *-0.5 *15 *((phi_beta *phi_beta - phi_beta *phi_beta *phi_beta) *(phi_liq - phi_alpha))+(-1.0/4.0 *(mu - B↔ _liq) *(mu - B_liq)/A+D_liq) *0.25 *15 *(3.0 *phi_liq *phi_liq *phi_liq *phi_liq - 4.0 *phi_liq *phi_liq *phi_liq - phi liq *phi liq +2.0 *phi liq -(phi alpha - phi beta) *(phi alpha - phi beta) *(2.0 *phi liq - 3.0 *phi liq *phi liq)))+(1.0/3.0) *(-2.0 *gamma *epsilon *dimx *dimx *fvc::laplacian(phi beta)+9.0 *gamma/epsilon *2.0 *(phi beta) *(1.0-phi beta) *(1.0-2.0 *phi beta) +(-1.0/4.0 *(mu - B alpha) *(mu - B alpha)/A+D alpha) *-0.5 *15 *((phi alpha *phi alpha - phi alpha *phi alpha *phi alpha) *(phi beta - phi liq))+(-1.0/4.0 *(mu -B beta) *(mu - B beta)/A+D beta) *0.25 *15 *(3.0 *phi beta *phi beta *phi beta *phi beta *phi beta - 4.0 *phi beta *phi_beta *phi_beta - phi_beta *phi_beta +2.0 *phi_beta -(phi_liq - phi_alpha) *(phi_liq - phi_alpha) *(2.↔ 0 *phi_beta - 3.0 *phi_beta *phi_beta))+(-1.0/4.0 *(mu - B_liq) *(mu - B_liq)/A+D_liq) *-0.5 *15 *((phi_liq *phi_liq - phi_liq *phi_liq *phi_liq) *(phi_beta - phi_alpha))))
- fvScalarMatrix phi_betaEqn (tau *epsilon *dimt *fvm::ddt(phi_beta) v *grad_beta.component(vector ::X)==(-2.0/3.0) *(-2.0 *gamma *epsilon *dimx *dimx *fvm::laplacian(phi_beta)+9.0 *gamma/epsilon *2.0 *(phi_beta) *(1.0-phi_beta) *(1.0-2.0 *phi_beta)+(-1.0/4.0 *(mu B_alpha) *(mu B_alpha)/A+D_alpha) *-0.5 *15 *((phi_alpha *phi_alpha phi_alpha *phi_alpha *phi_alpha) *(phi_beta phi_liq))+(-1.0/4.0 *(mu B_beta) *(mu B_beta)/A+D_beta) *0.25 *15 *(3.0 *phi_beta *phi_beta *phi_beta *phi_beta *phi_beta 4.0 *phi_beta *phi_beta *phi_beta phi_alpha) *(phi_liq phi_alpha) *(2. ← 0 *phi_beta 3.0 *phi_beta *phi_beta *phi_beta *phi_beta *phi_beta *phi_beta *phi_liq *phi_li

B_alpha) *(mu - B_alpha)/A+D_alpha) *-0.5 *15 *((phi_alpha *phi_alpha *phi_alpha *phi_alpha *phi_alpha) *(phi_liq - phi_beta))+(-1.0/4.0 *(mu - B_beta) *(mu - B_beta)/A+D_beta) *-0.5 *15 *((phi_beta *phi_beta *phi_beta *phi_beta *phi_beta) *(phi_liq - phi_alpha))+(-1.0/4.0 *(mu - B_liq) *(mu - B_liq)/A+D_liq) *0.25 *15 *(3.0 *phi_liq *phi_liq

- fvScalarMatrix phi liqEqn (tau *epsilon *dimt *fvm::ddt(phi liq) v *grad liq.component(vector::X)==(-2. 0/3.0) *(-2.0 *gamma *epsilon *dimx *dimx *fvm::laplacian(phi_liq)+9.0 *gamma/epsilon *2.0 *(phi_liq) *(1.0-phi_liq) *(1.0-2.0 *phi_liq)+(-1.0/4.0 *(mu - B_alpha) *(mu - B_alpha)/A+D_alpha) *-0.5 *15 *((phi alpha *phi alpha - phi alpha *phi alpha *phi alpha) *(phi liq - phi beta))+(-1.0/4.0 *(mu - B ↔ beta) *(mu - B_beta)/A+D_beta) *-0.5 *15 *((phi_beta *phi_beta - phi_beta *phi_beta *phi_beta *phi_beta) *(phi_liq - phi_alpha))+(-1.0/4.0 *(mu - B_liq) *(mu - B_liq)/A+D_liq) *0.25 *15 *(3.0 *phi_liq *phi_liq *phi_liq *phi_liq - 4.0 *phi_liq *phi_liq *phi_liq - phi_liq *phi_liq+2.0 *phi_liq -(phi_alpha - phi_beta) *(phi_alpha - phi beta) *(2.0 *phi liq - 3.0 *phi liq *phi liq)))+(1.0/3.0) *(-2.0 *gamma *epsilon *dimx *dimx *fvc↔ ::laplacian(phi alpha)+9.0 *gamma/epsilon *2.0 *(phi alpha) *(1.0-phi alpha) *(1.0-2.0 *phi alpha)+(-1.↔ 0/4.0 *(mu - B_alpha) *(mu - B_alpha)/A+D_alpha) *0.25 *15 *(3.0 *phi_alpha *phi_alpha *phi_alpha *phi_alpha - 4.0 *phi_alpha *phi_alpha *phi_alpha - phi_alpha *phi_alpha +2.0 *phi_alpha -(phi_beta - phi_liq) *(phi_beta - phi_liq) *(2.0 *phi_alpha - 3.0 *phi_alpha *phi_alpha))+(-1.0/4.0 *(mu - B_beta) *(mu - B_beta)/A+D_beta) *-0.5 *15 *((phi_beta *phi_beta - phi_beta *phi_beta *phi_beta) *(phi_alpha phi_liq))+(-1.0/4.0 *(mu - B_liq) *(mu - B_liq)/A+D_liq) *-0.5 *15 *((phi_liq *phi_liq - phi_liq *phi_liq *phi_liq) *(phi alpha - phi beta)))+(1.0/3.0) *(-2.0 *gamma *epsilon *dimx *dimx *fvc::laplacian(phi beta)+9.↔ 0 *gamma/epsilon *2.0 *(phi beta) *(1.0-phi beta) *(1.0-2.0 *phi beta)+(-1.0/4.0 *(mu - B alpha) *(mu -B alpha)/A+D alpha) *-0.5 *15 *((phi alpha *phi alpha - phi alpha *phi alpha *phi alpha) *(phi beta phi liq))+(-1.0/4.0 *(mu - B beta) *(mu - B beta)/A+D beta) *0.25 *15 *(3.0 *phi beta *phi beta *phi beta *phi beta - 4.0 *phi beta *phi beta *phi beta - phi beta *phi beta+2.0 *phi beta -(phi liq - phi alpha) *(phi liq - phi alpha) *(2.0 *phi beta - 3.0 *phi beta *phi beta))+(-1.0/4.0 *(mu - B liq) *(mu - B liq)/A+D↔ _liq) *-0.5 *15 *((phi_liq *phi_liq - phi_liq *phi_liq *phi_liq) *(phi_beta - phi_alpha))))
- while ((initial_residual_alpha.value() > Tol||initial_residual_beta.value() > Tol||initial_residual_liq.value() > Tol) &&counter< 100)

Variables

- dimensionedScalar initial_residual_alpha = phi_alphaEqn.solve().max().initialResidual()
- dimensionedScalar initial residual beta = phi betaEqn.solve().max().initialResidual()
- dimensionedScalar initial residual liq = phi liqEqn.solve().max().initialResidual()
- scalar counter = 0
- do
- volVectorField grad_beta =dimx*fvc::grad(phi_beta)
- volVectorField grad_liq =dimx*fvc::grad(phi_liq)

3.5.1 Function Documentation

3.5.1.1 phi_alphaEqn()

3.5.1.2 phi_betaEqn()

```
tau *epsilon *dimt * fvm::ddtphi_beta) - v *grad_beta.component(vector::X = =(-2.0/3.0) *(-2.0 *gostalentation *gostalentation
```

3.5.1.3 phi_liqEqn()

3.5.1.4 while()

```
while ( )
```

3.5.2 Variable Documentation

3.5.2.1 initial residual alpha

```
initial_residual_alpha = phi_alphaEqn.solve().max().initialResidual()
```

Definition at line 2 of file phi_abl_antiT.H.

3.5.2.2 initial_residual_beta

```
initial_residual_beta = phi_betaEqn.solve().max().initialResidual()
```

Definition at line 3 of file phi abl antiT.H.

3.5.2.3 initial residual liq

```
initial_residual_liq = phi_liqEqn.solve().max().initialResidual()
```

Definition at line 4 of file phi_abl_antiT.H.

3.5.2.4 counter

```
counter = 0
```

Definition at line 5 of file phi_abl_antiT.H.

3.5.2.5 do

do

Initial value:

```
volVectorField grad_alpha =dimx*fvc::grad(phi_alpha)
```

Implicit discretization using fvm class for time derivative and laplacian. Explicit discretization using fvc class for gradient and divergence. Phase-field equations with approximate relation between c, mu and T according to the parabolic approximation for free energy

Definition at line 9 of file phi_abl_antiT.H.

3.5.2.6 grad_beta

```
volVectorField grad_beta =dimx*fvc::grad(phi_beta)
```

Definition at line 11 of file phi_abl_antiT.H.

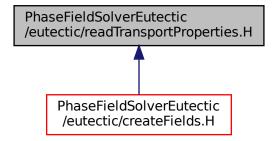
3.5.2.7 grad liq

```
volVectorField grad_lig =dimx*fvc::grad(phi_lig)
```

Definition at line 12 of file phi_abl_antiT.H.

3.6 PhaseFieldSolverEutectic/eutectic/readTransportProperties.H File Reference

This graph shows which files directly or indirectly include this file:



Functions

• IOdictionary transportProperties (IOobject("transportProperties", runTime.constant(), mesh, IOobject::←
MUST READ, IOobject::NO WRITE))

The input properties to be exported to createFields.

dimensionedScalar dimt (transportProperties.lookup("dimt"))

The input properties are read from constant/transportProperties dictionary.

dimensionedScalar dimx (transportProperties.lookup("dimx"))

Dimension of position.

dimensionedScalar ms_alpha (transportProperties.lookup("ms_alpha"))

Slope liq-alpha and alpha-liq.

• dimensionedScalar ms beta (transportProperties.lookup("ms beta"))

Slope liq-beta and beta-liq.

• dimensionedScalar c_eq_liq (transportProperties.lookup("c_eq_liq"))

Eutectic composition of liquid phase.

• dimensionedScalar c_eq_alpha (transportProperties.lookup("c_eq_alpha"))

Eutectic composition of alpha phase.

dimensionedScalar c_eq_beta (transportProperties.lookup("c_eq_beta"))

Eutectic composition of beta phase.

• dimensionedScalar G (transportProperties.lookup("G"))

Thermal gradient.

dimensionedScalar v (transportProperties.lookup("v"))

Velocity.

- dimensionedScalar A (transportProperties.lookup("A"))
- dimensionedScalar D (transportProperties.lookup("D"))

Diffusivity in liquid.

• dimensionedScalar T_eut (transportProperties.lookup("T_eut"))

Eutectic temperature.

• dimensionedScalar initial (transportProperties.lookup("initial"))

Constant value from temperature profile.

• dimensionedScalar tau (transportProperties.lookup("tau"))

Relaxation coefficient.

• dimensionedScalar gamma (transportProperties.lookup("gamma"))

Interface energy parameter.

• dimensionedScalar epsilon (transportProperties.lookup("epsilon"))

Interface width parameter.

3.6.1 Function Documentation

3.6.1.1 transportProperties()

The input properties to be exported to createFields.

3.6.1.2 dimt()

The input properties are read from constant/transportProperties dictionary.

Dimension of time

3.6.1.3 dimx()

```
\label{local_dimx} \mbox{dimensionedScalar dimx (} \\ \mbox{transportProperties. } \mbox{lookup"dimx"})
```

Dimension of position.

Referenced by main().

Here is the caller graph for this function:



3.6.1.4 ms_alpha()

```
\label{limits} {\tt dimensionedScalar\ ms\_alpha\ (} \\ {\tt transportProperties.} \quad {\tt lookup"ms\_alpha"\ )}
```

Slope liq-alpha and alpha-liq.

Referenced by main().



3.6.1.5 ms_beta()

Slope liq-beta and beta-liq.

Referenced by main().

Here is the caller graph for this function:



3.6.1.6 c_eq_liq()

```
dimensioned
Scalar c_eq_liq ( transport Properties. \ \ lookup \mbox{\it "c}\_eq\_liq \mbox{\it "}\ )
```

Eutectic composition of liquid phase.

Referenced by main().

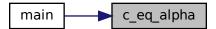


3.6.1.7 c_eq_alpha()

Eutectic composition of alpha phase.

Referenced by main().

Here is the caller graph for this function:



3.6.1.8 c_eq_beta()

Eutectic composition of beta phase.

Referenced by main().



3.6.1.9 G()

```
dimensioned
Scalar G ( transportProperties. \ \ lookup \text{\it "G"} \ )
```

Thermal gradient.

Referenced by main().

Here is the caller graph for this function:



3.6.1.10 v()

```
dimensioned
Scalar v ( {\tt transportProperties.} \quad {\tt lookup"v"} \; )
```

Velocity.

3.6.1.11 A()

```
dimensioned
Scalar A ( transport \texttt{Properties.} \quad \textit{lookup"A"} \ )
```

Referenced by main().



3.6.1.12 D()

```
dimensionedScalar D ( transportProperties. \quad lookup \textit{"D"} \ )
```

Diffusivity in liquid.

3.6.1.13 T_eut()

Eutectic temperature.

Referenced by main().

Here is the caller graph for this function:



3.6.1.14 initial()

Constant value from temperature profile.

Referenced by main().



3.6.1.15 tau()

```
\label{local_continuous} \mbox{dimensionedScalar tau (} \\ \mbox{transportProperties. } \mbox{lookup"tau"})
```

Relaxation coefficient.

3.6.1.16 gamma()

Interface energy parameter.

3.6.1.17 epsilon()

Interface width parameter.

3.7 PhaseFieldSolverEutectic/eutectic/set_delta_t.H File Reference

Functions

runTime setDeltaT (min(deltaTFactor *runTime.deltaTValue(), maxDeltaT))

Variables

dimensionedScalar maxResidual = 1e-7

Timestep reduction for improving convergence.

- dimensionedScalar maxDeltaT = 1
- dimensionedScalar maxDeltaTFactor = maxResidual/(initial_residual_liq)
- dimensionedScalar deltaTFactor = min(min(maxDeltaTFactor, 1.0 + 0.1*maxDeltaTFactor), 1. ← 2*(maxDeltaTFactor/maxDeltaTFactor))

3.7.1 Function Documentation

3.7.1.1 setDeltaT()

3.7.2 Variable Documentation

3.7.2.1 maxResidual

```
dimensionedScalar maxResidual = 1e-7
```

Timestep reduction for improving convergence.

Definition at line 36 of file set_delta_t.H.

3.7.2.2 maxDeltaT

```
dimensionedScalar maxDeltaT = 1
```

Definition at line 37 of file set_delta_t.H.

3.7.2.3 maxDeltaTFactor

```
dimensionedScalar maxDeltaTFactor = maxResidual/( initial_residual_liq)
```

Definition at line 38 of file set_delta_t.H.

3.7.2.4 deltaTFactor

```
\label{eq:dimensionedScalar} $$ \mbox{deltaTFactor} = \min(\min(\max DeltaTFactor, 1.0 + 0.1*\max DeltaTFactor), 1.$$ $$ 2*(\max DeltaTFactor/\max DeltaTFactor)) $$
```

Definition at line 39 of file set_delta_t.H.

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