

An easy-to-use calphad tool – CALPHAD CAE

Chunhui Luo*

*Currently working at Swerim AB, Sweden

Contents

Introduction

Schematic of CALPHAD CAE software structure

Installing and running Calphad CAE

Software GUI

Thermodynamic modeling by using Pycalphad

Process modeling by using Kawin (Precipitation)

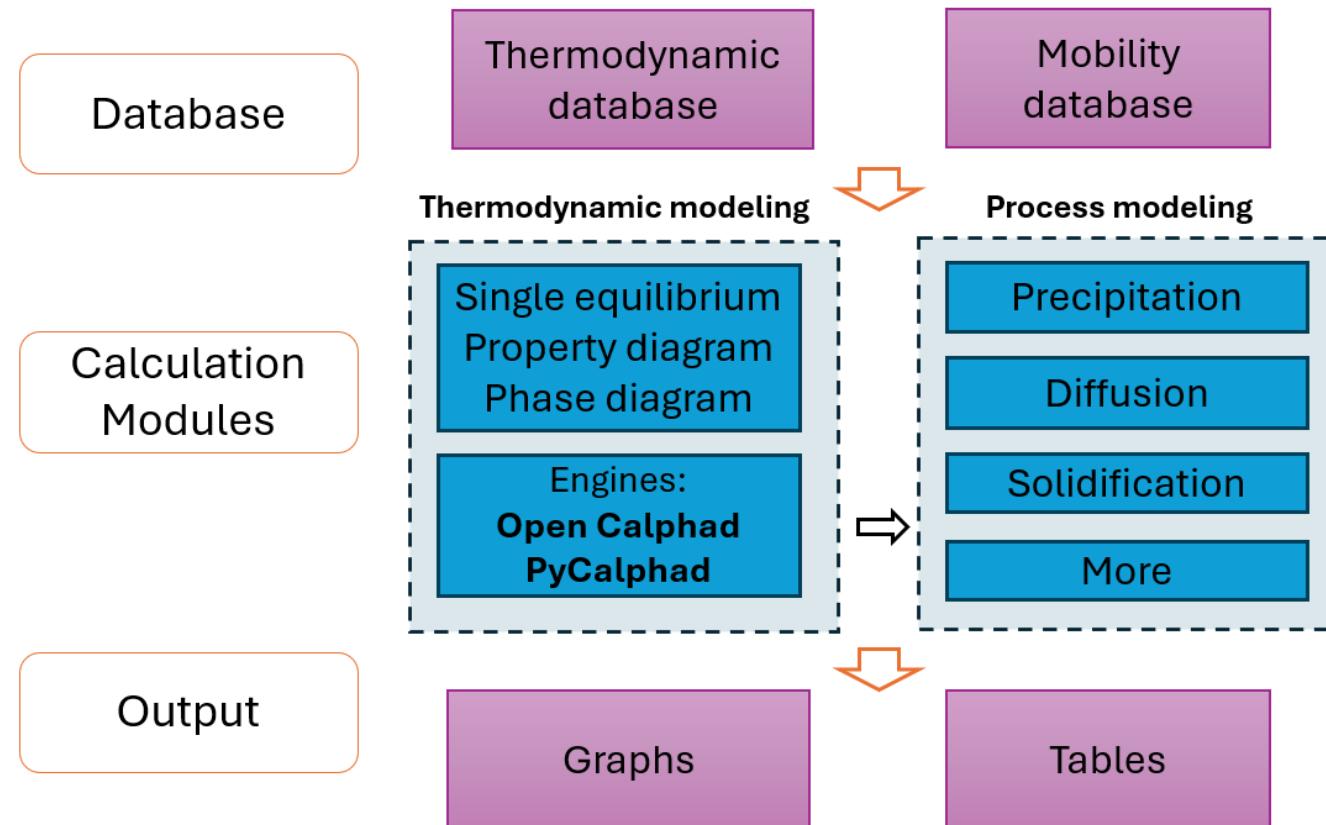
Quick demo



Introduction

- Open-source Calphad tools (Opencalphad using macro script; pycalphad using python) requires user to have a Calphad background and programming skills.
- **Calphad CAE** is a graphical user interface (GUI) designed to simplify the use and development of Calphad applications based on both Open Calphad and Pycalphad. Additionally, Calphad CAE is enhanced for kinetic processes using open-source software such as Kawin, collectively referred to as Calphad CA Advanced.
- Developing histories:
 - ❑ 2018 started to develop GUI for OpenCalphad -> Opencalphad CAE
 - ❑ 2023 started to develop GUI for pycalphad and kawin -> Calphad CAE
- Use python and PySide2 as GUI developing tool, deliver stand-alone code to user (Windows only for the moment)
- Project management: save and save as a project, open and modify an exiting project

Schematic of CALPHAD CAE software structure



Installing and running Calphad CAE

Download:

<https://www.dropbox.com/scl/fo/0zikeb0ssedp0i11z38tl/AGRqq4anar4de-dClF7P9wo?rlkey=majcmoplebua0hux7s2dadzu1&dl=0>

Install: **Calphad_CAE_Setup_ver0_0_1.exe** (Windows)

Default installation location: C:\Calphad_CAE_0_0_1

Double-click

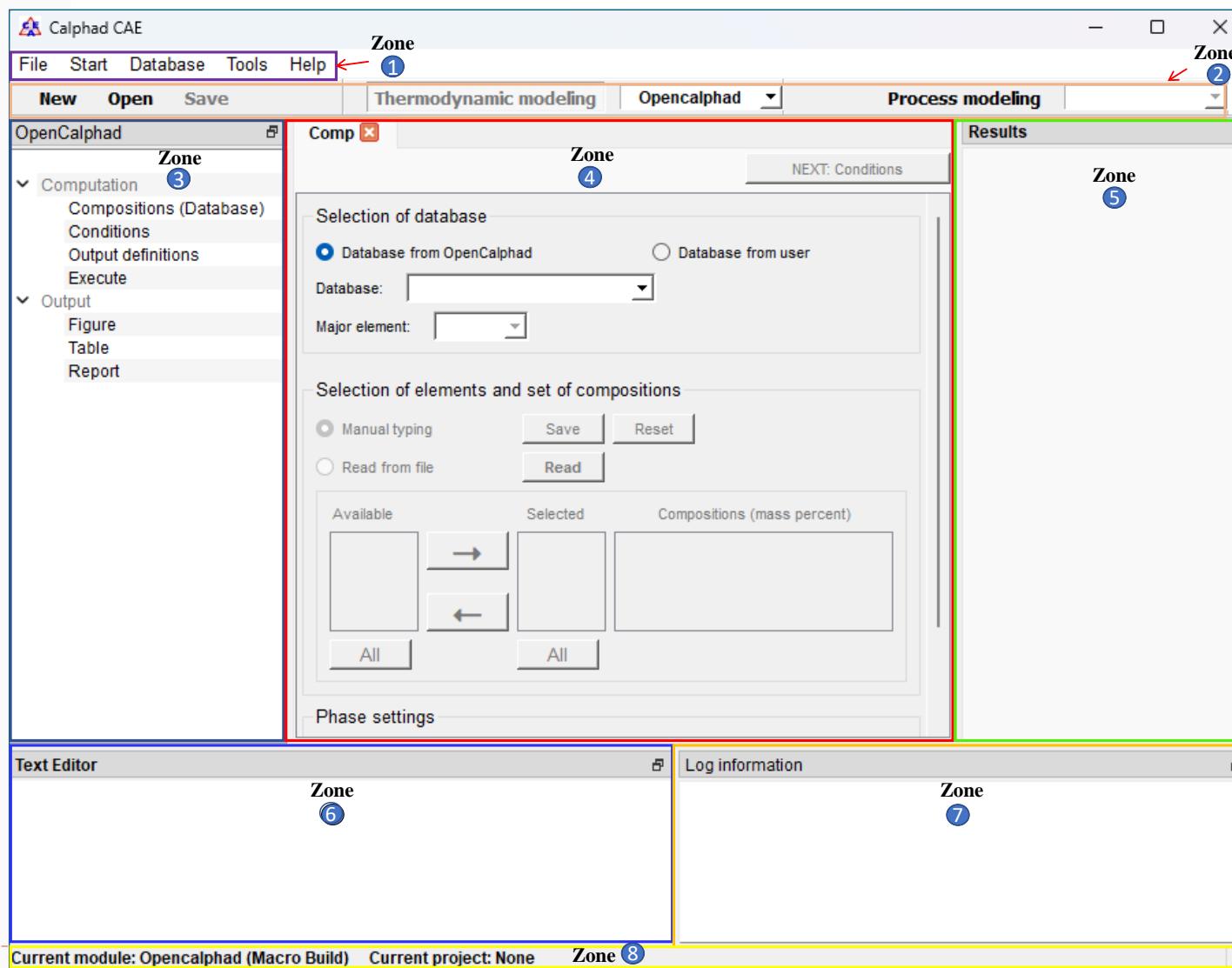


Uninstall:



From C:\Calphad_CAE_0_0_1

GUI layout



Zone 1: Menus

Zone 2: Toolbars

Zone 3: Task tree

Zone 4: Task definitions

Zone 5: Results

Zone 6: Text editor

Zone 7: Log information

Zone 8: Status bar

Thermodynamic modeling by using Pycalphad

Example: property diagram

Comp X **Cond** X **Exec** X

6 NEXT: Conditions **10** NEXT: Execute **17** NEXT: Figure

Selection of database

From OpenCalphad **1** From Pycalphad From user

Database: iron4cd **2**

Major element: FE **3**

Selection of elements and set of compositions

Manual typing

Read from file **4**

Save Reset

Read **5** FeCMnSi.json

Available	Selected	Compositions (mass percent)
CR	C	Element Mass percent
CU	MN	C 0.1
MG	SI	MN 1.5
MO		SI 0.3
N		FE 98.1
NB		
NI		
TI		
V		

6 NEXT: Conditions

Calc 1 +

Define calculation type

Single equilibrium Property diagram **7** Phase diagram Advanced

Conditions

Temperature: Kelvin **1000**

Pressure: Pascal **101325**

System size: Mole **1**

Composition	Mass percent
Composition C	0.1
Composition MN	1.5
Composition SI	0.3

Phase selection **7**

Phase

Available phases(31)

- B2_BCC **8**
- C14_LAVES
- C15_LAVES
- I_BCC_A2
- I_CEMENTITE_D011
- CBCC_A12
- FCC_A1
- LIQUID
- CR3SI_A15
- CR5Si3_D8M
- CRSi2_C40
- M23C6_D84
- M5C2
- M7C3_D101

Selected phases(7)

- BCC_A2
- CEMENTITE_D011
- FCC_A1
- LIQUID
- M23C6_D84
- M5C2
- M7C3_D101

9

Current diagram: Property diagram

Define variable 1

Axis variable: Temperature **10**

Min: 300.0 Max: 2000.0 Step: 1

Execute Pycalphad modeling

Select calculation: **Calc 1** **11**

Calculation state: Calculation completed

Plot results after calculation

Options for Calc1:

Use phase selection in Cond **12**

Start calculation **13**

Save project

Project Name: pycalphad_propertydiagram_FeCMnSi **14**

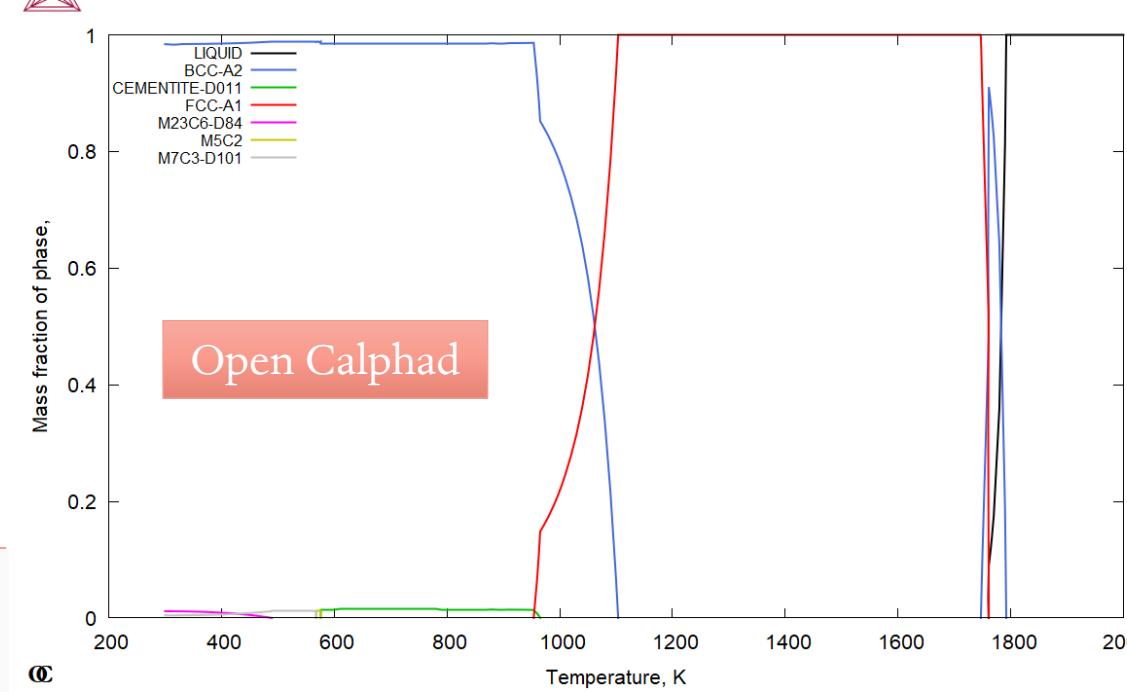
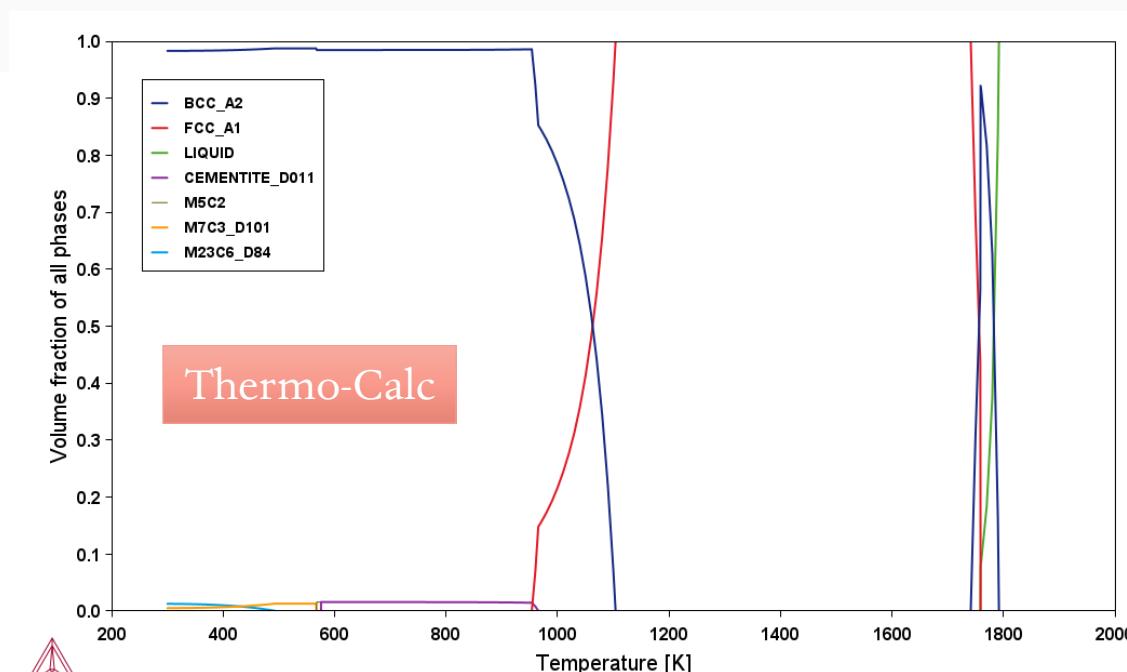
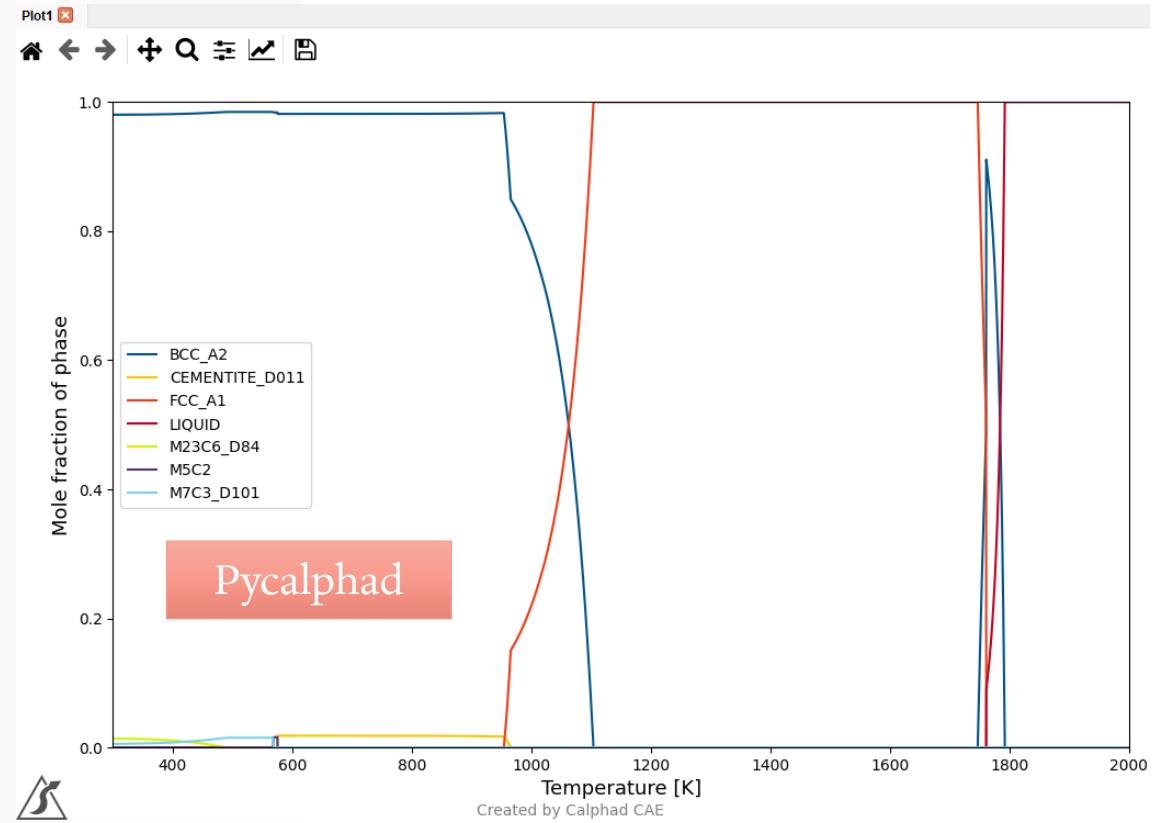
Create **15**

Project directory: C:/Calphad_CAE_0_0_1/results/Pycalphad/pycalphad_propertydiagram_FeCMnSi

Save project **16** copy user database to project folder

Show project file (*.json)

**Example: property diagram
(Fe-0.1C-1.5Mn-0.3Si alloy, wt%)**



Process modeling by using Kawin (Precipitation)

Example: Multiphase precipitation in Al-Mg-Si system

Comp 7 **NEXT: Conditions**

Selection of database
 From OpenCalphad From Kawin 1 From user
 Database: AlMgSi 2 Mobility data included
 Database (mobility): <Import user database>
 Major element: AL 3

Selection of elements and set of compositions
 Manual typing 4 Read from file
 Save Reset
 Read

Available	Selected	Compositions (mole fraction)
MG	→	AL Mole fraction 0.9871
SI	←	MG Mole fraction 0.0072 5
All	All	SI Mole fraction 0.0057 6

Comp **Cond** NEXT: Execute

Calc 1 +

Composition

1 Composition MG	Mole fraction	0.0072	
2 Composition SI	Mole fraction	0.0057	

Matrix phase

Phase: FCC_A1 8
 Molar volume: 1.0E-5 9 m³/mol
 Grain size: 100 μm
 Grain aspect ratio: 1.0
 Dislocation density: 1E12 10 m⁻²
 Driving force method: Approximate
 Mobility correction: Same for all elements Correction factor: 1
 Elastic properties: None

Precipitate phases

+ 15 Phase: MGSI_B_P 11 (1)
 Molar volume: 1.0E-5 12 m³/mol
 Nucleation sites: Dislocations 13
 Calculate nucleation sites 3.919646643145e+21 m⁻³
 Shape: Sphere
 Transformation strain: None
 Interfacial energy: 0.18 14 J/m²

Comp **Cond** **Exec** 52 NEXT: Figure

Execute precipitation simulation

Select calculation: Calc 1 46

Calculation state: Calculation completed

Save results to CSV file
 Plot results after simulation 47

More settings:

Calc1: Number of iterations to print status: 100
 time for size distribution: 25.0
 Sampling density for equilibrium calculations: 500
 Sampling density for driving force: 2000
 Model solver: Explicit Euler

Start simulation 48

Save project

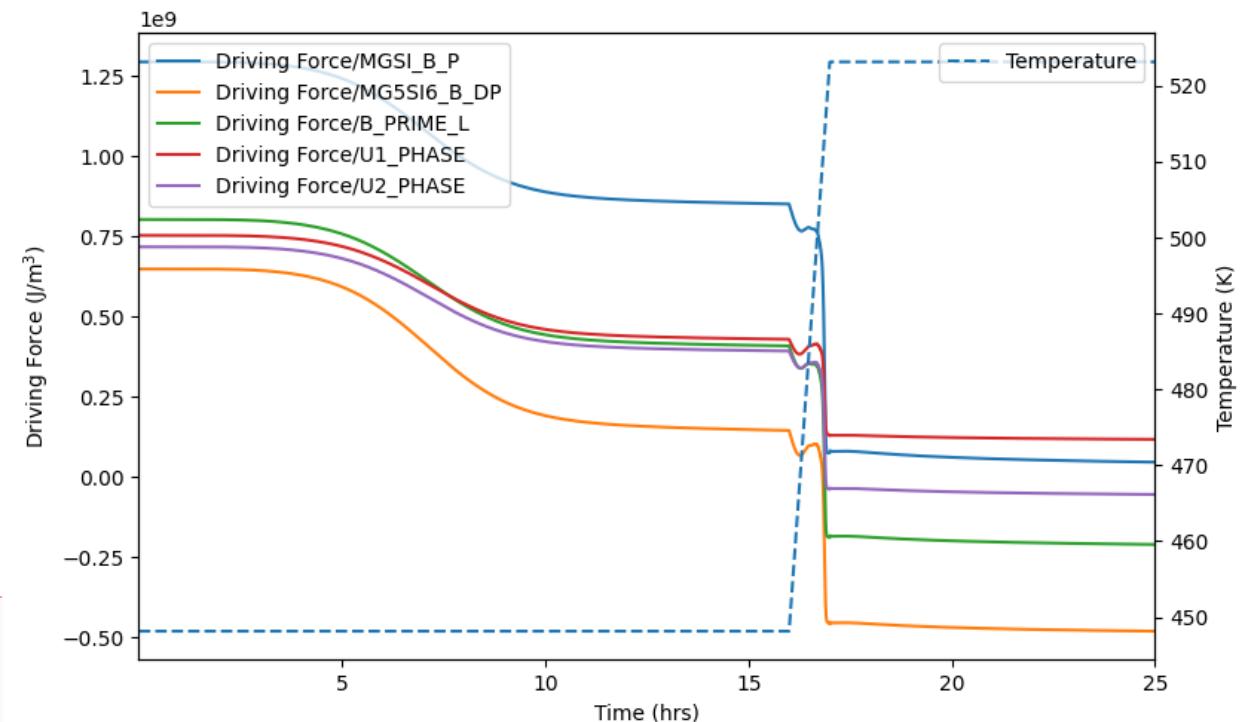
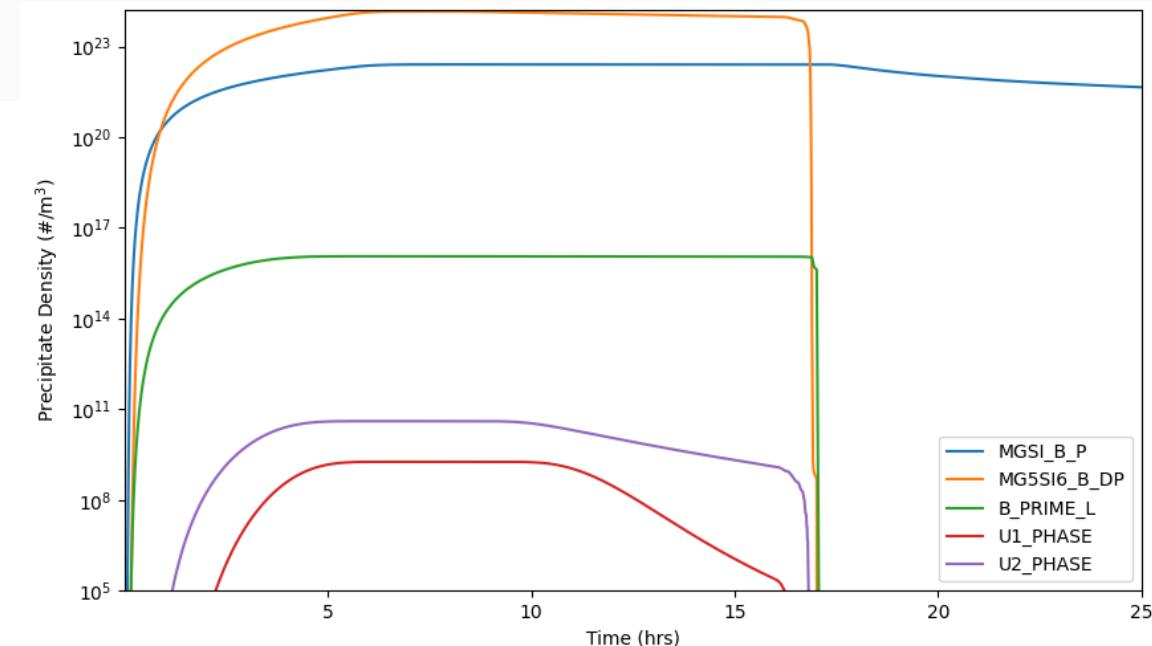
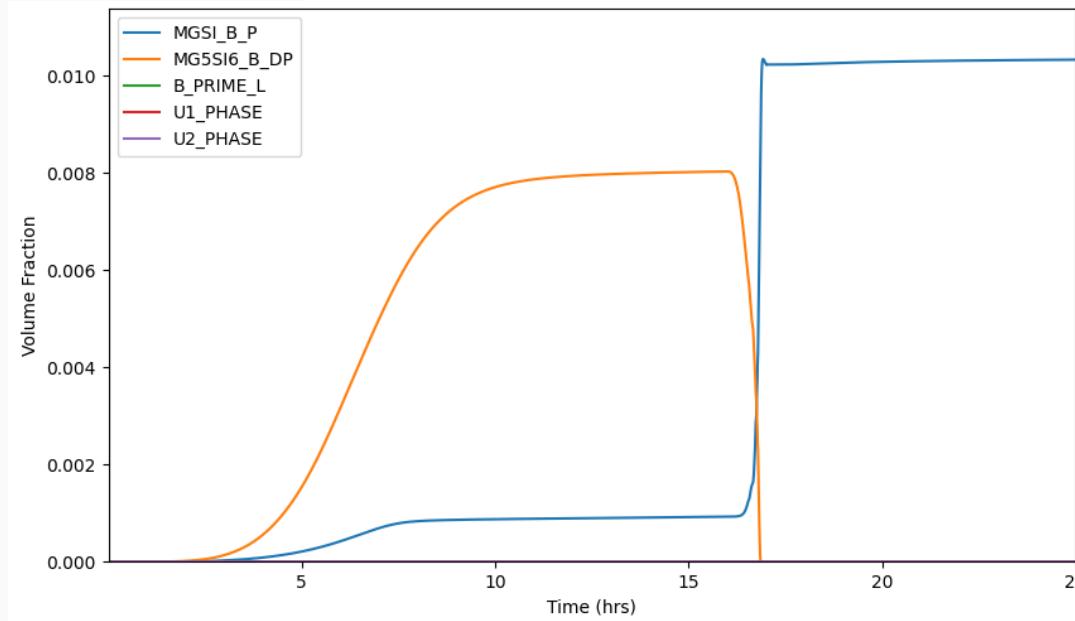
Project Name: precip_AlMgSi_5phase_Nonisothermal 49 New Create 50

Project directory: C:/Calphad_CAE_0_0_1/results/Precipitation/precip_AlMgSi_5phase_Nonisothermal

Save project 51 copy user database to project folder

Show project file (*.json)

Example: Multiphase precipitation in Al-Mg-Si system



Thank You !

Now start demonstration