ICAMS
INTERDISCIPLINARY CENTRE FOR ADVANCED MATERIALS SIMULATION

Project group: Deformation and Phase Transformations.

OpenPhase - the open source phase field simulation package.

Department "Scale Bridging and Thermodynamic Simulation".
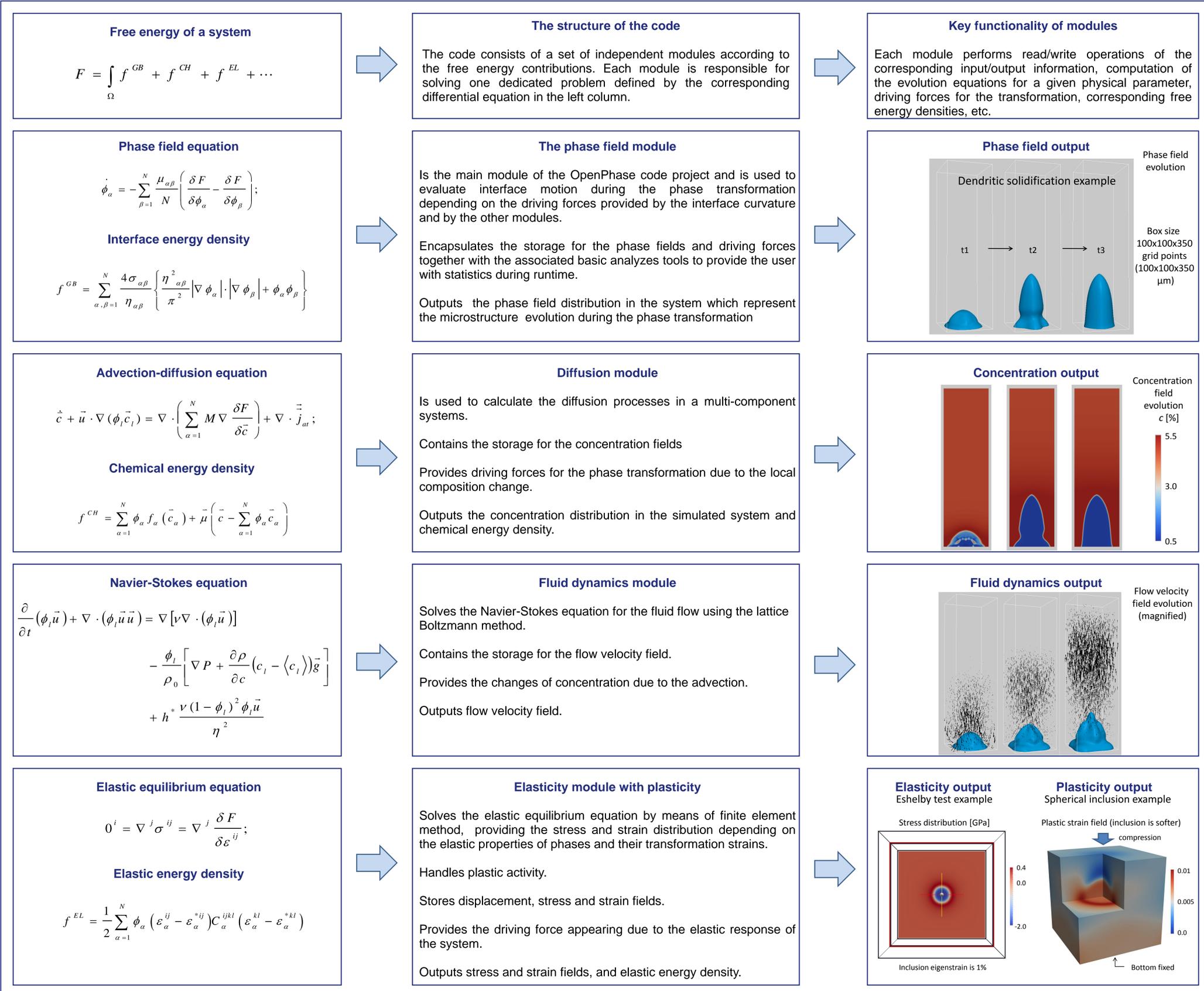
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The main aim of the project

… is to enable researchers from ICAMS and in the near future from all over the world to perform high quality *quantitative* simulations of microstructure formation during phase transformations

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Free energy of a system

$$F = \int_{\Omega} f^{GB} + f^{CH} + f^{EL} + \cdots$$

The structure of the code

The code consists of a set of independent modules according to the free energy contributions. Each module is responsible for solving one dedicated problem defined by the corresponding differential equation in the left column.

Key functionality of modules

Each module performs read/write operations of the corresponding input/output information, computation of the evolution equations for a given physical parameter, driving forces for the transformation, corresponding free energy densities, etc.

Phase field equation

$$\dot{\phi}_\alpha = -\sum_{\beta=1}^{N} \frac{\mu_{\alpha\beta}}{N} \left(\frac{\delta F}{\delta \phi_\alpha} - \frac{\delta F}{\delta \phi_\beta} \right);$$

Interface energy density

$$f^{GB} = \sum_{\alpha,\beta=1}^{N} \frac{4\sigma_{\alpha\beta}}{\eta_{\alpha\beta}} \left\{ \frac{\eta^2_{\alpha\beta}}{\pi^2} |\nabla \phi_\alpha| \cdot |\nabla \phi_\beta| + \phi_\alpha \phi_\beta \right\}$$

The phase field module

Is the main module of the OpenPhase code project and is used to evaluate interface motion during the phase transformation depending on the driving forces provided by the interface curvature and by the other modules.

Encapsulates the storage for the phase fields and driving forces together with the associated basic analyzes tools to provide the user with statistics during runtime.

Outputs the phase field distribution in the system which represent the microstructure evolution during the phase transformation

Phase field output

Phase field evolution

Dendritic solidification example

t1 → t2 → t3

Box size 100x100x350 grid points (100x100x350 μm)

Advection-diffusion equation

$$\dot{\vec{c}} + \vec{u} \cdot \nabla (\phi_l \vec{c}_l) = \nabla \cdot \left(\sum_{\alpha=1}^{N} M \nabla \frac{\delta F}{\delta \vec{c}} \right) + \nabla \cdot \vec{j}_{at};$$

Chemical energy density

$$f^{CH} = \sum_{\alpha=1}^{N} \phi_\alpha f_\alpha (\bar{c}_\alpha) + \bar{\mu} \left(\bar{c} - \sum_{\alpha=1}^{N} \phi_\alpha \bar{c}_\alpha \right)$$

Diffusion module

Is used to calculate the diffusion processes in a multi-component systems.

Contains the storage for the concentration fields

Provides driving forces for the phase transformation due to the local composition change.

Outputs the concentration distribution in the simulated system and chemical energy density.

Concentration output

Concentration field evolution c [%]

5.5

3.0

0.5

Navier-Stokes equation

$$\frac{\partial}{\partial t} (\phi_l \vec{u}) + \nabla \cdot (\phi_l \vec{u}\vec{u}) = \nabla [\nu \nabla \cdot (\phi_l \vec{u})]$$

$$- \frac{\phi_l}{\rho_0} \left[\nabla P + \frac{\partial \rho}{\partial c} (c_l - \langle c_l \rangle) \vec{g} \right]$$

$$+ h^* \frac{\nu (1 - \phi_l)^2 \phi_l \vec{u}}{\eta^2}$$

Fluid dynamics module

Solves the Navier-Stokes equation for the fluid flow using the lattice Boltzmann method.

Contains the storage for the flow velocity field.

Provides the changes of concentration due to the advection.

Outputs flow velocity field.

Fluid dynamics output

Flow velocity field evolution (magnified)

Elastic equilibrium equation

$$0^i = \nabla^j \sigma^{ij} = \nabla^j \frac{\delta F}{\delta \varepsilon^{ij}};$$

Elastic energy density

$$f^{EL} = \frac{1}{2} \sum_{\alpha=1}^{N} \phi_\alpha \left(\varepsilon^{ij}_\alpha - \varepsilon^{*ij}_\alpha \right) C^{ijkl}_\alpha \left(\varepsilon^{kl}_\alpha - \varepsilon^{*kl}_\alpha \right)$$

Elasticity module with plasticity

Solves the elastic equilibrium equation by means of finite element method, providing the stress and strain distribution depending on the elastic properties of phases and their transformation strains.

Handles plastic activity.

Stores displacement, stress and strain fields.

Provides the driving force appearing due to the elastic response of the system.

Outputs stress and strain fields, and elastic energy density.

Elasticity output
Eshelby test example

Stress distribution [GPa]

0.4
0.0

-2.0

Inclusion eigenstrain is 1%

Plasticity output
Spherical inclusion example

Plastic strain field (inclusion is softer)

compression

0.01

0.005

0.0

Bottom fixed

Further development of the OpenPhase

Will be focused on:
- extension of the model for the case of plastic activity during the phase transformation,
- linking to the CALPHAD type databases for retrieving of the Gibbs free energies of the phases,
- heat transfer problem solver,
- MPI parallelization of the code,
- further development of the underlying multi-phase field model

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Official web page
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General information about the OpenPhase

- based on the multi-phase field multi-component model [1],
- object oriented code written in C++ programming language,
- modular structure allowing for easy extension by adding of new modules,
- supports serial and OpenMP parallel execution environments,
- at the current state consists of almost 20 000 lines of code,
- will be distributed in the form of open and free of charge source code,
- paid support can be provided per request for inexperienced external users.

[1] I.Steinbach, Modeling Simul. Mater. Sci. Eng., 17 (2009) 073001