Allen-Cahn in MOOSE

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1 Introduction

Energy functional F.

$$F = \int_{\Omega} f(\eta) + \frac{\kappa}{2}\nabla^2\eta dV \tag{1}$$

Free energy density.

$$f(\eta) = 2\eta^2(1-\eta)^2 - 0.2\eta \tag{2}$$

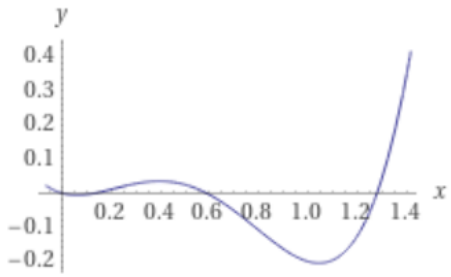

Figure 1: Equation 2 for the free energy density.

Allen-Cahn equation.

$$\frac{\delta\eta}{\delta t} = -L\mu \tag{3}$$

The chemical potential of the system is given by the variational derivative of the energy functional F.

$$\mu = \frac{\delta F}{\delta\eta} = \frac{\delta f}{\delta\eta} - \kappa\nabla^2\eta \tag{4}$$

The Allen-Cahn equation becomes,

$$\frac{\delta\eta}{\delta t} = -L\left(\frac{\delta f}{\delta\eta} - \kappa\nabla^2\eta\right) \tag{5}$$

2 Weak formulation for FEM

1. Multiply with test-function w and integrate over the system.

$$\int_{\omega} \frac{\delta \eta}{\delta t} \cdot w + L\left(\frac{\delta f}{\delta \eta} - \kappa \nabla^2 \eta\right) \cdot w dV = 0 \tag{6}$$

$$\int_{\omega} \frac{\delta \eta}{\delta t} \cdot w + L\frac{\delta f}{\delta \eta} \cdot w - L\kappa \nabla^2 \eta \cdot w dV = 0 \tag{7}$$

2. Integrate the parts involving partial derivatives using Green's formula (integration by parts) to reduce the order of derivatives.

$$\int_{\omega} \frac{\delta \eta}{\delta t} \cdot w + L\frac{\delta f}{\delta \eta} \cdot w + L\kappa \nabla \eta \cdot \nabla w dV = 0 \tag{8}$$

Now, the whole expression is solved in MOOSE by dividing the three terms into their appropriate kernels

Kernel 1 (TimeDerivative)

$$\left(\frac{\delta \eta}{\delta t}, w\right) \tag{9}$$

Kernel 2 (AllenCahn)

$$\left(L\frac{\delta f}{\delta \eta}, w\right) \tag{10}$$

Kernel 3 (ACInterface)

$$\left(L\kappa \nabla \eta, \nabla w\right) \tag{11}$$

```
[Kernels]
  [./eta]
    type =  TimeDerivative
    variable = eta
  []

  [./ACBulk]
    type = AllenCahn
    variable = eta
    f_name = F
    mob_name = 1.0
  [../]

  [./ACint]
  type = ACInterface
  variable = eta
  mob_name = 1.0
  kappa_name = 0.5
[../]
[]
```