工业中的多尺度力学方法

相场方法算例讲解

主讲人：倪勇 教授

助　教: 陆宇阳

日　期: 2021.01.15







概要

- 调幅分解过程模拟
- 多晶生长过程模拟
- 晶体相场方法模拟结构相变
- 断裂相场方法模拟裂纹扩展

调幅分解过程模拟

目的：演示经典相场方法中经典的Cahn-Hilliard方程模拟相分离过程

Cahn-Hilliard 方程：

$$\frac{\partial c(\mathbf{r},t)}{\partial t} = M\nabla^2 \frac{\delta F_{tot}}{\delta c(\mathbf{r},t)} + \xi(\mathbf{r},t)$$

C: 浓度　　M: 迁移率　　扰动

总能量：$F_{tot} = F_{loc} + F_{int}$

$$F_{loc} = \int_V f_c(c)\,dV \qquad F_{int} = \int_V \frac{1}{2}\nabla c \cdot \kappa \nabla c\,dV$$

Regular solution model:

$$f_c = \Omega c(1-c) + k_B T\left(c\ln c + (1-c)\ln(1-c)\right)$$

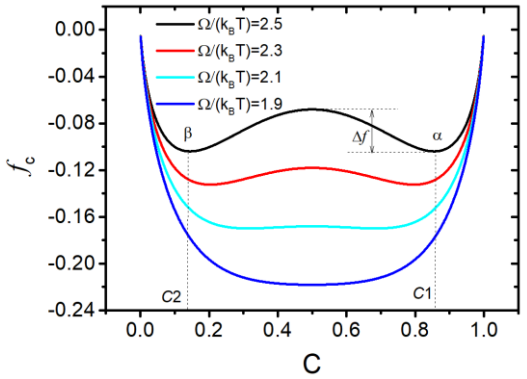
要点1：FFT（快速傅里叶变换）方法求解高阶偏微分方程

$$\tilde{F}\left[\frac{\partial f}{\partial x_i}\right] = ik_i\tilde{F}[f] \qquad k_i = \sin\left(\frac{2\pi s_i}{n_i}\right) \qquad \tilde{F}\left[\frac{\partial^2 f}{\partial x_i^2}\right] = -k_i^2\tilde{F}[f] \qquad k_i^2 = 2\left[1-\cos\left(\frac{2\pi s_i}{n_i}\right)\right]$$

要点2：Spinodal point的确定与初值设定的关系

$$c(x,t) = c_0 + \zeta\exp(\mathrm{i}q\,x + \sigma t)$$

$$\sigma = -M\left[\beta q^4 + \gamma q^2\right]$$



调幅分解过程模拟

离散实空间和傅里叶空间

```
n=256;
h=n;
x=linspace(1,h,n);
y=linspace(1,h,n);
xs=x(2)-x(1);
ys=y(2)-y(1);
fx=2*pi/xs;
fy=2*pi/ys;
kx=fx*(1:n)/n;
ky=fy*(1:n)/n;
vect=ones(n);
k2x=zeros(n,n);
k2y=zeros(n,n);
   for i=1:1:n;
   k2x(i,:)=kx(i)*vect(i,:);
   end
for i=1:1:n;
   k2y(:,i)=ky(i)*vect(:,i);
end
```

```
kkx=(-2*(cos(k2x)-1));
kky=(-2*(cos(k2y)-1));
```

$$k_i^2 = 2\left[1-\cos\left(\frac{2\pi s_i}{n_i}\right)\right]$$

初值

```
c0=0.5; %
c=c0+turbulence*(0.5-rand(n));
```

$$\frac{\partial \tilde{C}(\xi,t)}{\partial t} = -\xi^2 \tilde{f}^*(C(\xi,t)) - k^*\xi^4 \tilde{C}(\xi,t)$$

方程求解

```
p= wa*(1-2*c)+log(complex(c)./(1-complex(c)));
fc=fft2(c);  %
fp=fft2(p);
midc = (fc + unitt*(-kk.*fp-beta*kk.^2.*fc));
c=ifft2(midc);
c=real(c);
```

调幅分解过程模拟

程序提交

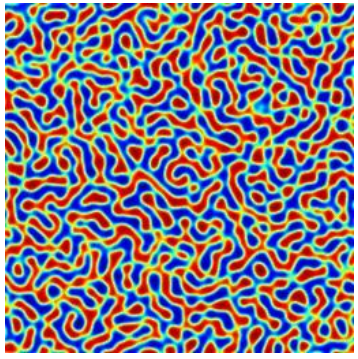
```
cd ~/WORK/students/online/
```

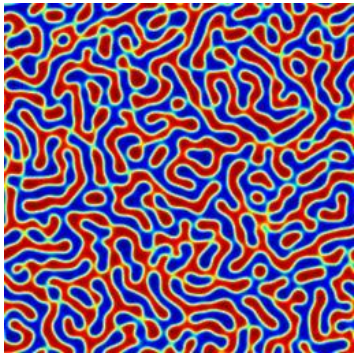
到自己的文件夹

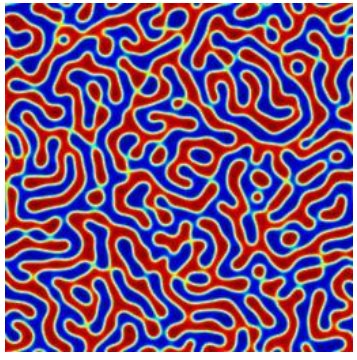
```
cp ~/WORK/winterschool/day5/phase_field_lyy/case1/{matlab_run.sh,p1.m} ./
```

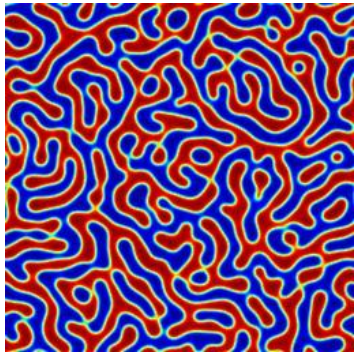
```
[train1@ln01 case1]$ sbatch matlab_run.sh
Submitted batch job 119693
```

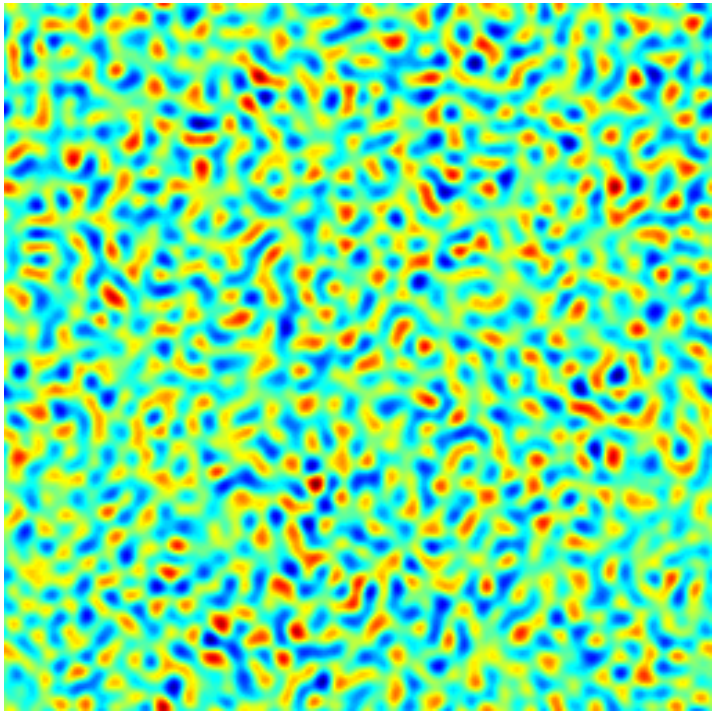
结果展示











多晶生长过程模拟

目的：讲授经典相场方法中经典的Allen-Cahn方程模拟多晶中晶粒生长过程

Allen-Cahn方程

$$\frac{\partial \eta_1(\mathbf{r},t)}{\partial t} = -\hat{L}_{1j}\frac{\delta F_{tot}}{\delta \eta_j(\mathbf{r},t)} + \xi_1(\mathbf{r},t)$$

…

$$\frac{\partial \eta_\theta(\mathbf{r},t)}{\partial t} = -\hat{L}_{\theta j}\frac{\delta F_{tot}}{\delta \eta_\theta(\mathbf{r},t)} + \xi_\theta(\mathbf{r},t)$$

序参量：$\eta_1(\mathbf{r},t),\ldots\eta_\theta(\mathbf{r},t)$　动力学系数：$\hat{L}_{1j}\cdots\hat{L}_{\theta j}$

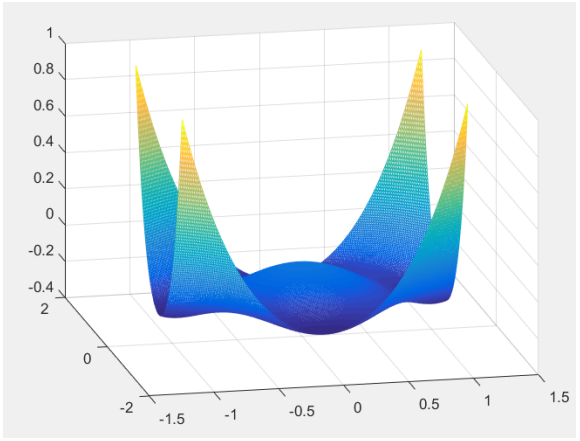
总能量：

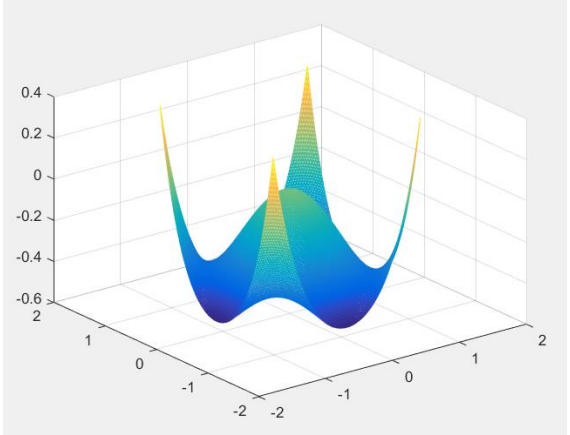
$$F^{\text{tot}}(t) = \int\left(f_0\left(\xi_q(\mathbf{r},t)\right) + \sum_{q=1}^{Q}\frac{\beta_q}{2}\left(\nabla\xi_q(\mathbf{r},t)\right)^2\right)d\mathbf{r}$$

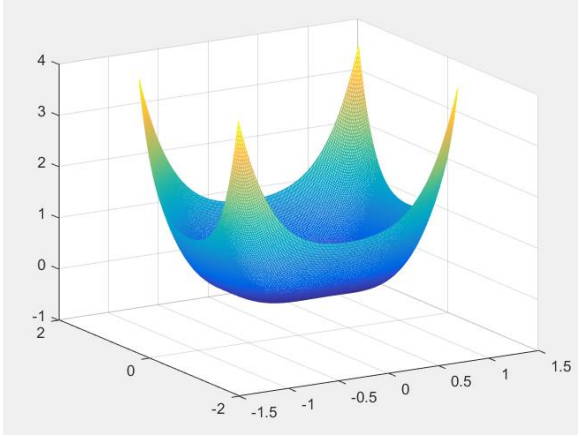
朗道自由能函数：

$$f_0\left(\xi_q(\mathbf{r},t)\right) = -\frac{\alpha_1}{2}\sum_{q=1}^{Q}\xi_q{}^2(\mathbf{r},t) + \frac{\alpha_2}{4}\left(\sum_{q=1}^{Q}\xi_q{}^2(\mathbf{r},t)\right)^2 + \left(\alpha_3 - \frac{\alpha_2}{2}\right)\sum_{q=1}^{Q}\sum_{s>q}^{Q}\xi_q{}^2(\mathbf{r},t)\xi_s{}^2(\mathbf{r},t),$$

要点：自由能函数朗道多项式的形式和设置







多晶生长过程模拟

初值

```
for m=1:1:p;
ax=round(rand(1,1)*nx);
ay=round(rand(1,1)*ny);
   for i = 1:1:nx;
       for j=1:1:ny;

        if round(sqrt((i-ax)^2+(j-ay)^2)) <= 15
                    eta(i,j,m)=1.0;
        end
       end
   end
end
```

方程

$$f_0\left(\xi_q(\mathbf{r},t)\right)=-\frac{\alpha_1}{2}\sum_{q=1}^{Q}\xi_q^{\,2}(\mathbf{r},t)+\frac{\alpha_2}{4}\left(\sum_{q=1}^{Q}\xi_q^{\,2}(\mathbf{r},t)\right)^2+\left(\alpha_3-\frac{\alpha_2}{2}\right)\sum_{q=1}^{Q}\sum_{s>q}^{Q}\xi_q^{\,2}(\mathbf{r},t)\xi_s^{\,2}(\mathbf{r},t),$$

$$\tilde{F}^{n+1}\left[\eta_1(\mathbf{r},t)\right]-\tilde{F}^{n}\left[\eta_1(\mathbf{r},t)\right]=-\Delta t\hat{L}_{1j}\left(\tilde{F}^{n}\left[\frac{\partial f_0}{\partial\eta_1(\mathbf{r},t)}\right]+\beta k^2\tilde{F}^{n+1}\left[\eta_1(\mathbf{r},t)\right]\right)$$

$$\left(1+\Delta t\hat{L}_{1j}\beta k^2\right)\tilde{F}^{n+1}\left[\eta_1(\mathbf{r},t)\right]=\tilde{F}^{n}\left[\eta_1(\mathbf{r},t)\right]-\Delta t\hat{L}_{1j}\tilde{F}^{n}\left[\frac{\partial f_0}{\partial\eta_1(\mathbf{r},t)}\right]$$

方程求解

```
s_eta2 = 0;
for m=1:1:p;
  s_eta2 = s_eta2 + eta(:,:,m).^2;
end
for g = 1:1:p;
    chem_eta(:,:,g) = -alfa1*eta(:,:,g)+alfa2*eta(:,:,g).^3 ...
        + 2*alfa3*eta(:,:,g).*(s_eta2-eta(:,:,g).^2);
    f_chem_eta(:,:,g)=fft2(chem_eta(:,:,g));
    f_eta(:,:,g)=fft2(eta(:,:,g));
    mid_feta(:,:,g)=(f_eta(:,:,g)-step*mobile.*f_chem_eta(:,:,g))./(1+step*mobile*beta*kk);
    eta(:,:,g)=real(ifft2(mid_feta(:,:,g)));%+raodong*(0.5-rand(nx,ny));
end
```

多晶生长过程模拟

程序提交

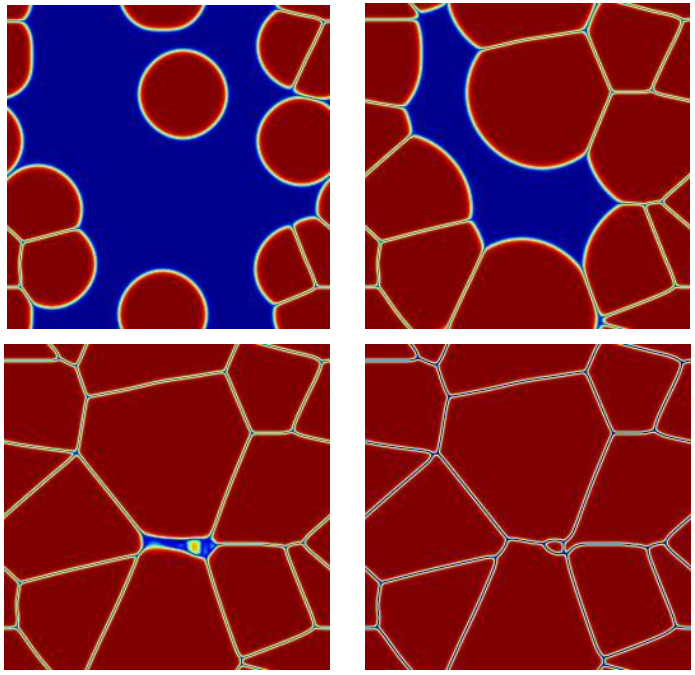
```
cd ~/WORK/students/online/
```

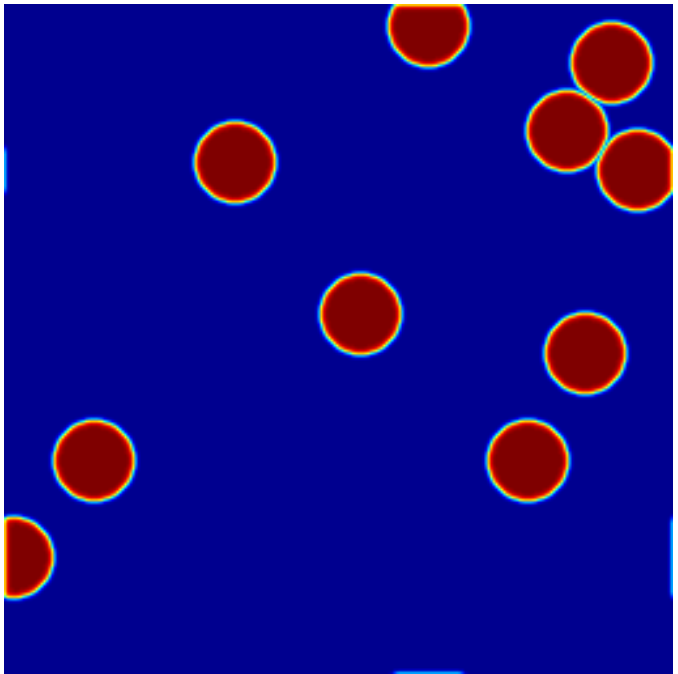
到自己的文件夹

```
case2]$ cp ~/WORK/winterschool/day5/phase_field_lyy/case2/{matlab_run.sh,g2.m} ./
```

```
[train1@ln01 case2]$ sbatch matlab_run.sh
Submitted batch job 119698
```

结果展示





晶体相场方法模拟结构相变

$$\frac{\partial \rho}{\partial t}=\left[\nabla^{10}+6\nabla^{8}+13\nabla^{6}+12\nabla^{4}+(4-\varepsilon)\nabla^{2}\right]\rho+\nabla^{2}\rho^{3}$$

```
f_lro=fft2(lro);
mid_flro = (f_lro-step*kk.*fft2(lro.^3))./...
(1-step*(-kk.^5+14/3*kk.^4-73/9*kk.^3+56/9*kk.^2-(16/9-epsilon)*kk));
lro=real(ifft2(mid_flro))+change*(0.5-rand(nx,ny));
```

程序提交

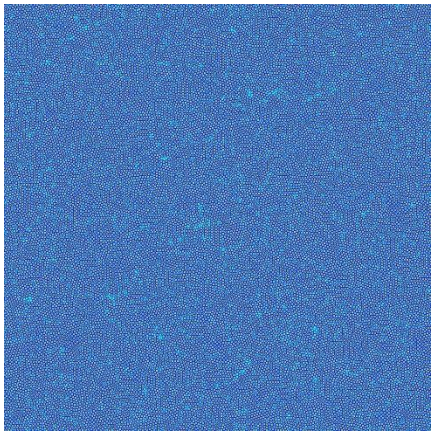
```
mkdir case3   cd ~/WORK/students/online/
```

到自己的文件夹

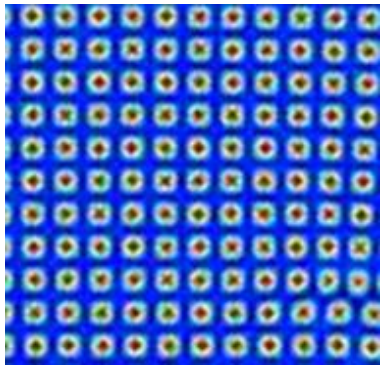
```
[train1@ln01 case3]$ cp ~/WORK/winterschool/day5/phase_field_lyy/case3/{matlab_run.sh,p3.m} .
[train1@ln01 case3]$ ls
matlab_run.sh  p3.m
```

```
[train1@ln01 case3]$ sbatch matlab_run.sh
Submitted batch job 119700
```

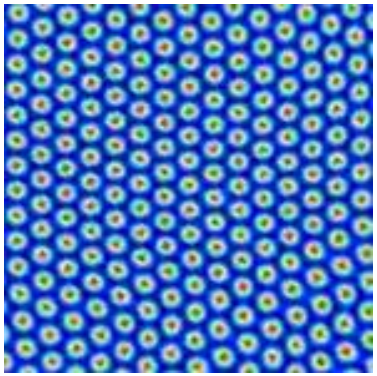
结果：



四方相：



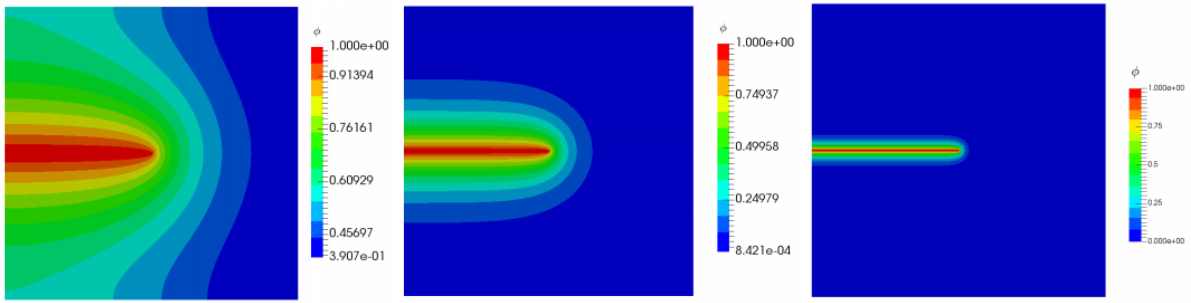
六方相：



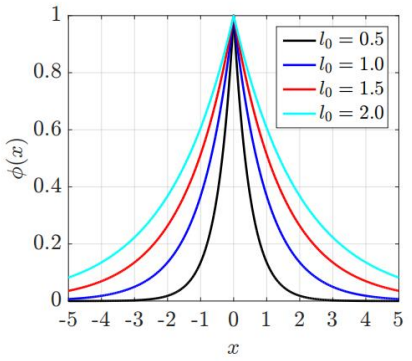
断裂相场方法模拟裂纹扩展

控制方程：$Y - G_c\,\delta_\phi\gamma = 0$

$$Y := -\frac{\partial\psi}{\partial\phi} = -\frac{\partial\psi}{\partial g}\frac{\partial g}{\partial\phi} = -g'(\phi)\bar{Y}, \qquad \bar{Y} := \frac{\partial\psi}{\partial g} \qquad \delta_\phi\gamma = \frac{1}{c_0}\left[\frac{1}{l_0}\alpha'(\phi) - 2l_0\Delta\phi\right]$$



$l_0 = \{0.5, 0.02, 0.05\}.$



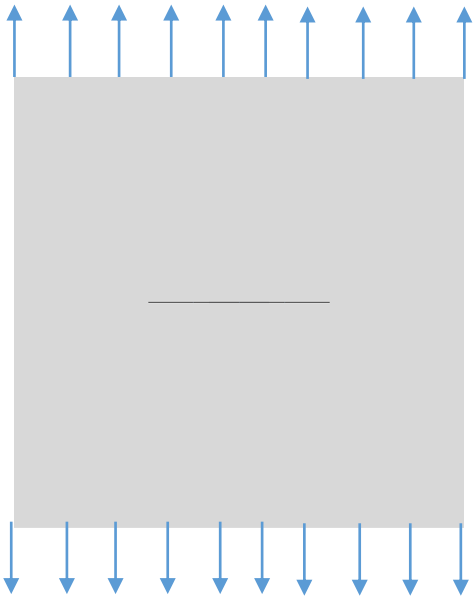
来源：Corrado Maurini，J.Y. Wu, C. Miehe，G. Molnár, Bourdin, Kuhn

断裂相场模型上机流程（ABAQUS）

1. ABAQUS建立模型，输出原始inp文件

2. 修改inp文件和编写for文件，再输入到ABAQUS中进行计算得到结果

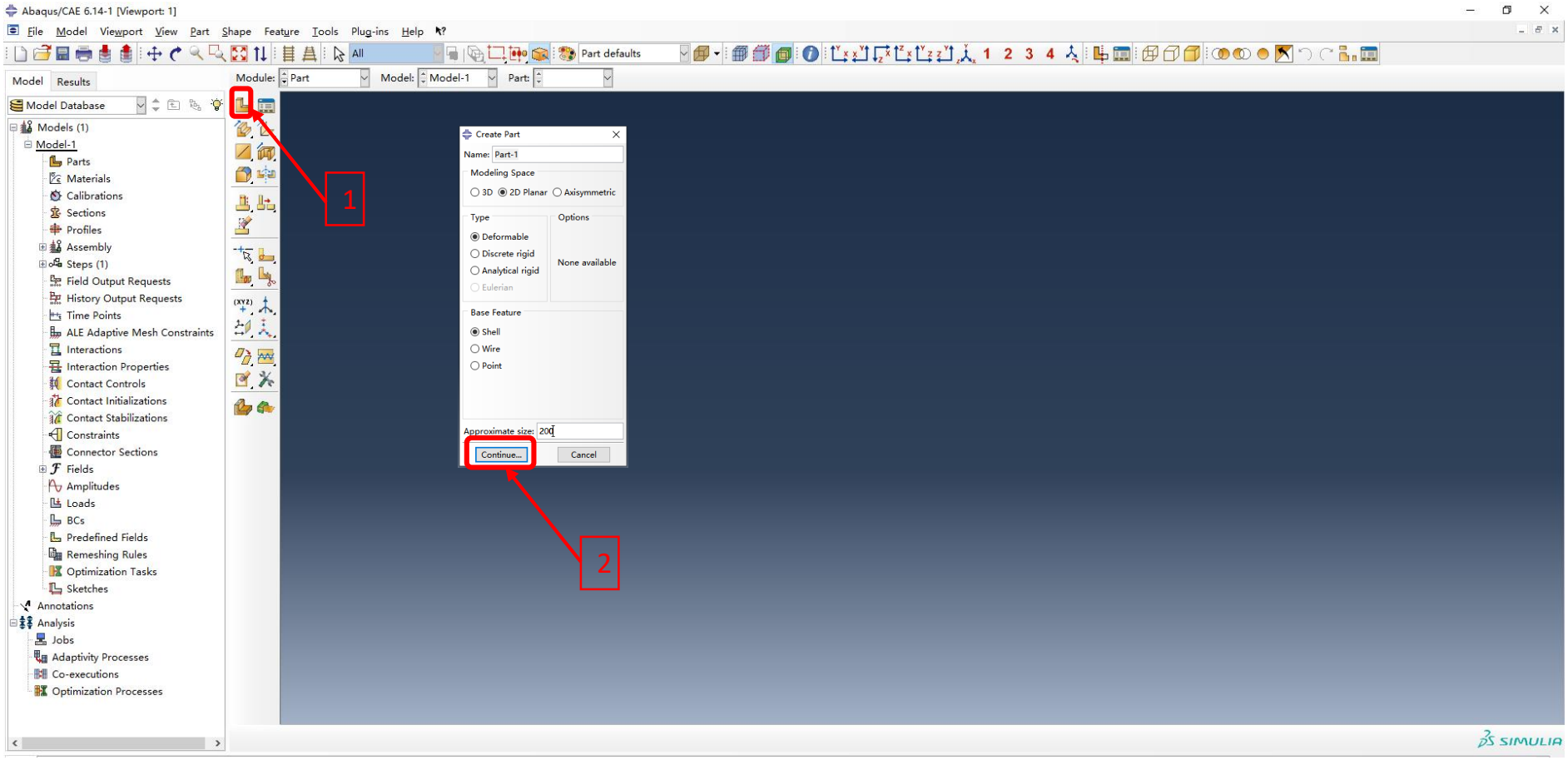
3. 用ABAQUS或者Paraview进行后处理



问题描述

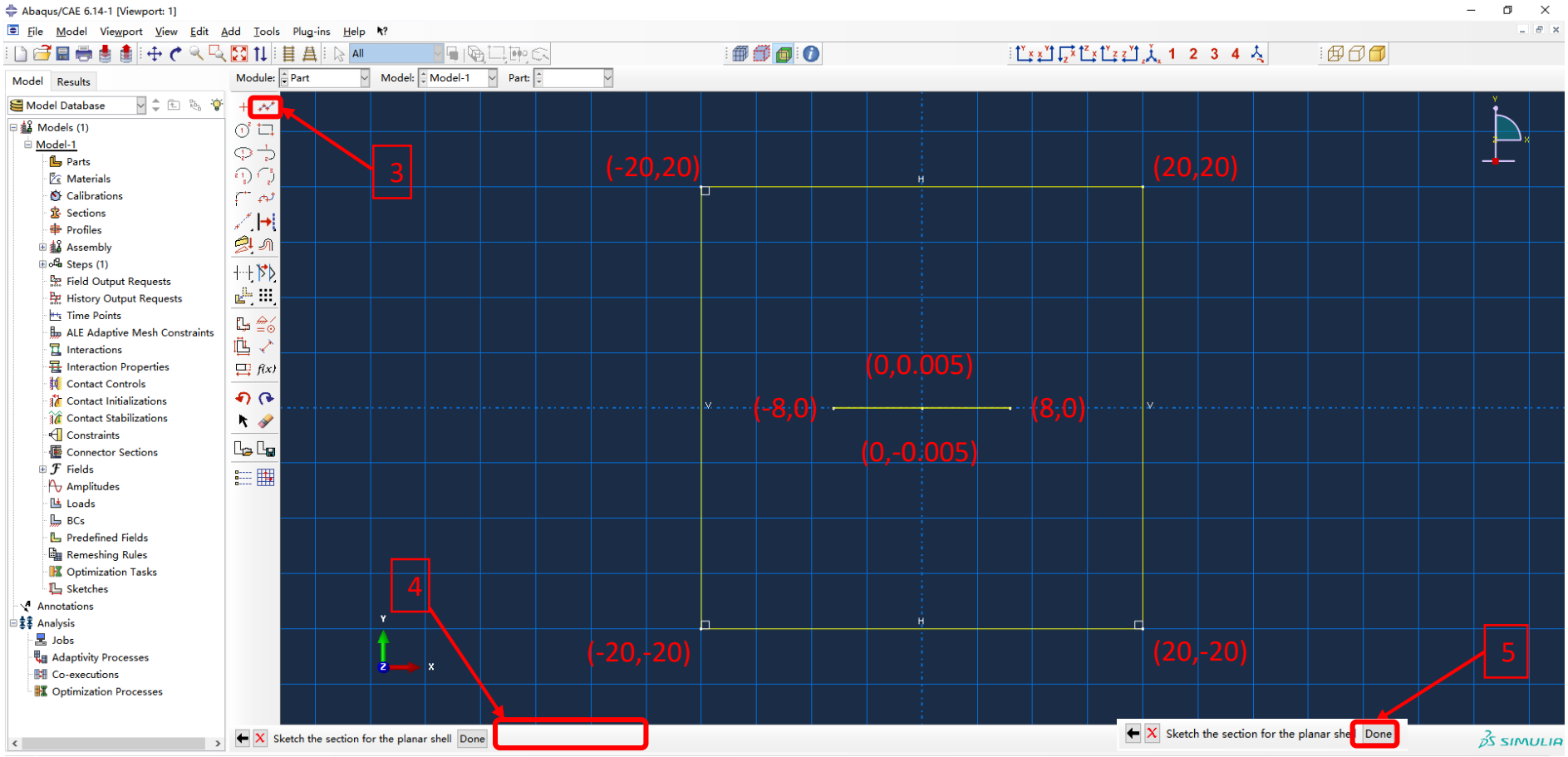
断裂相场方法模拟裂纹扩展

建模步骤（part）



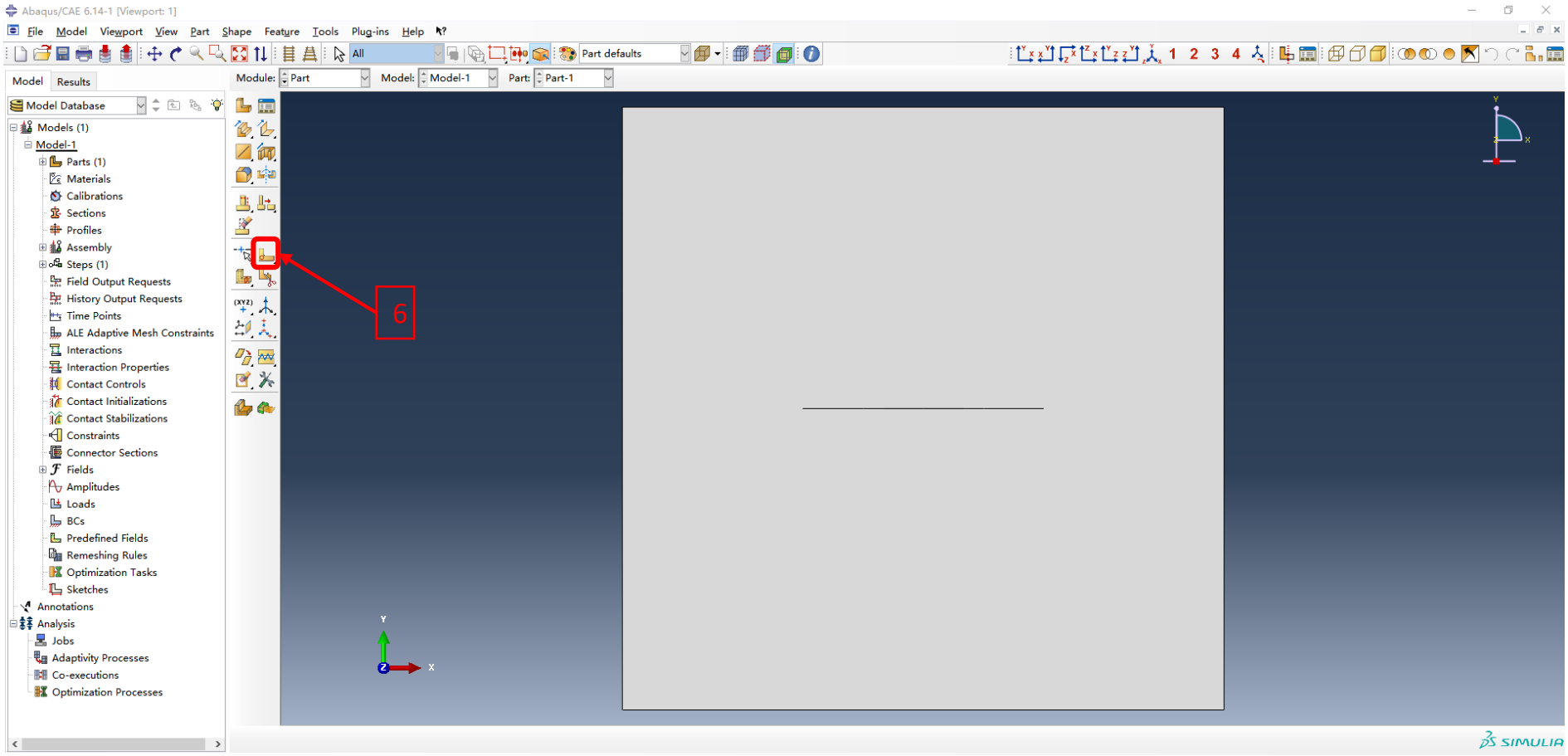
断裂相场方法模拟裂纹扩展

建模步骤（part）



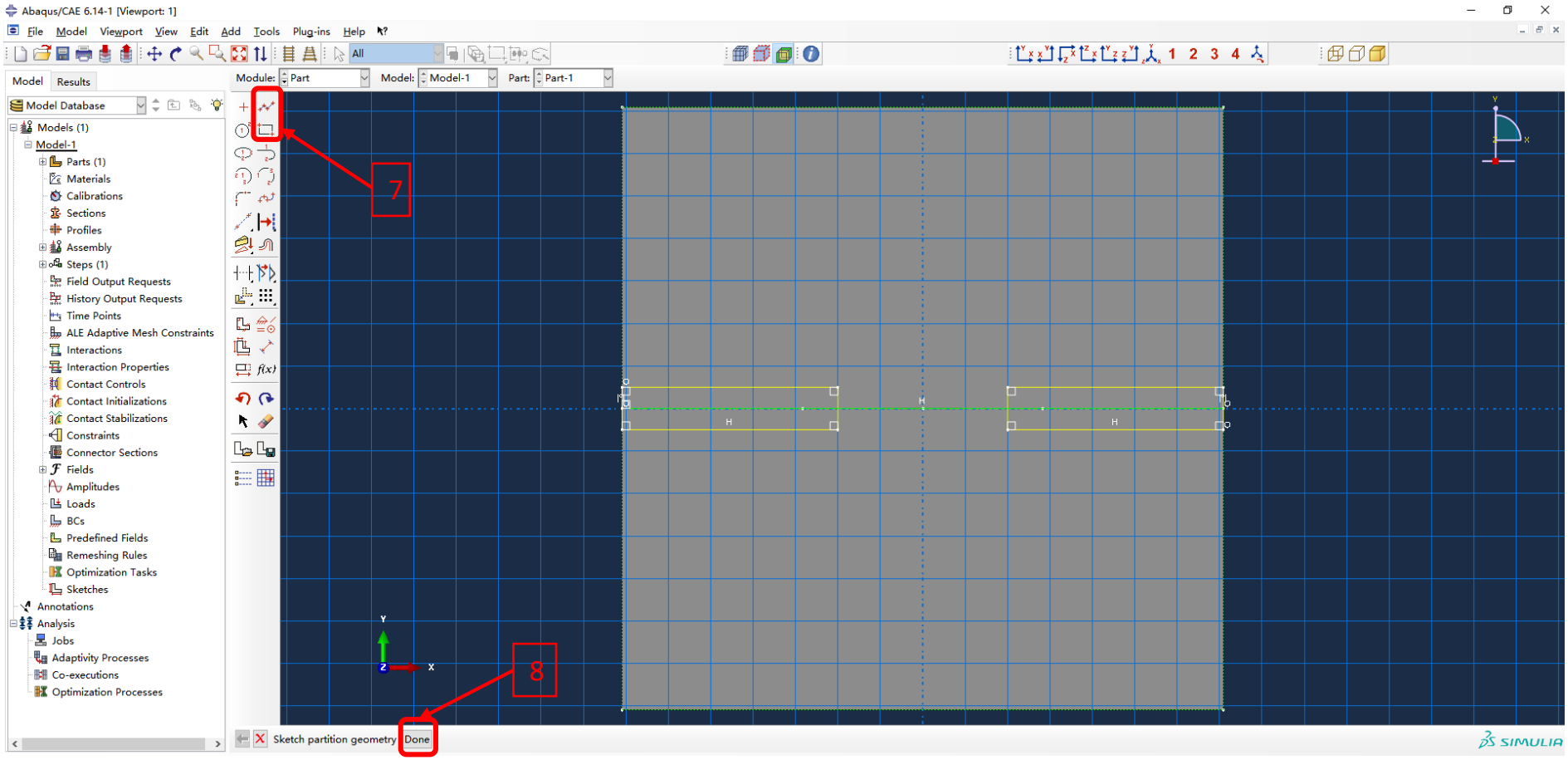
断裂相场方法模拟裂纹扩展

建模步骤（part）



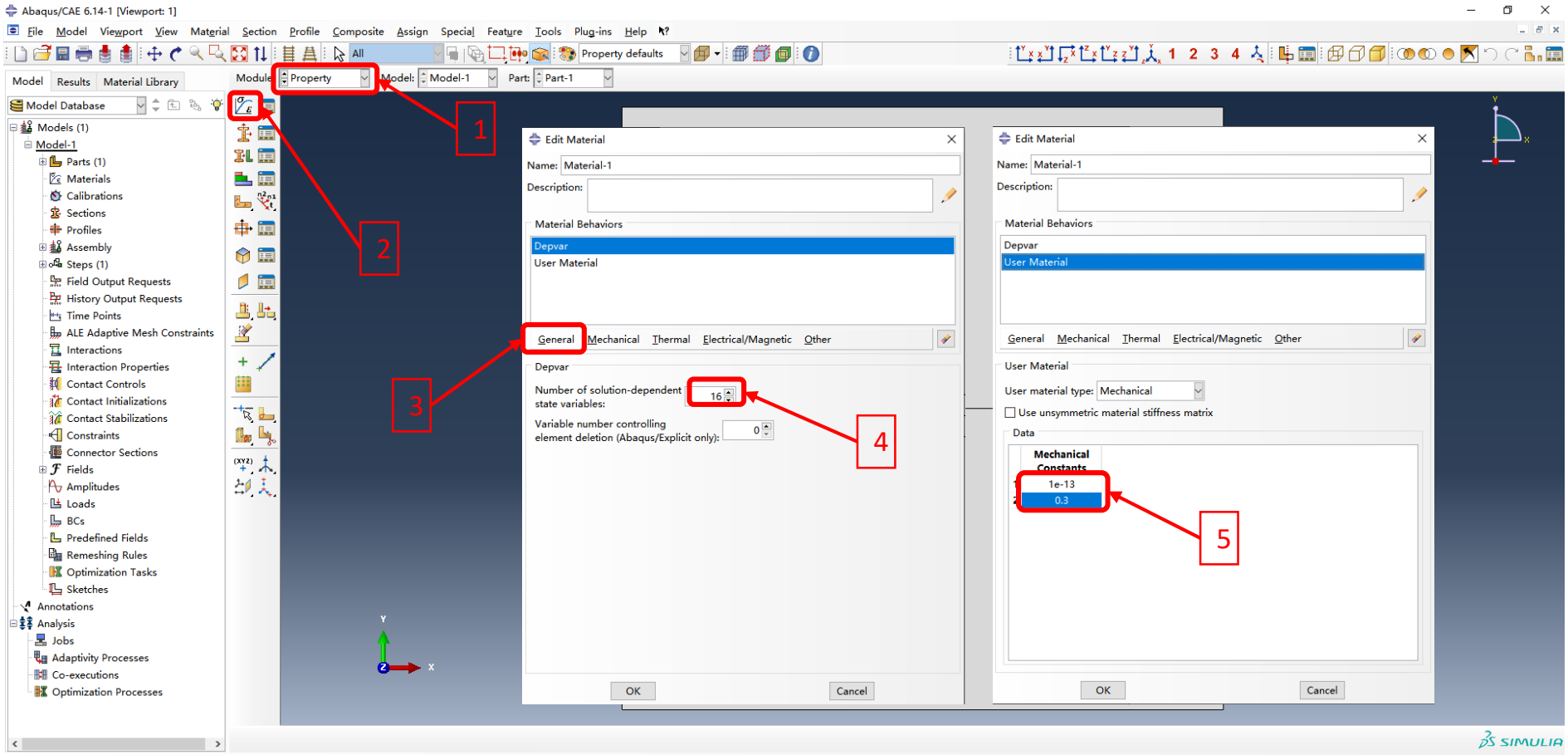
断裂相场方法模拟裂纹扩展

建模步骤（part）



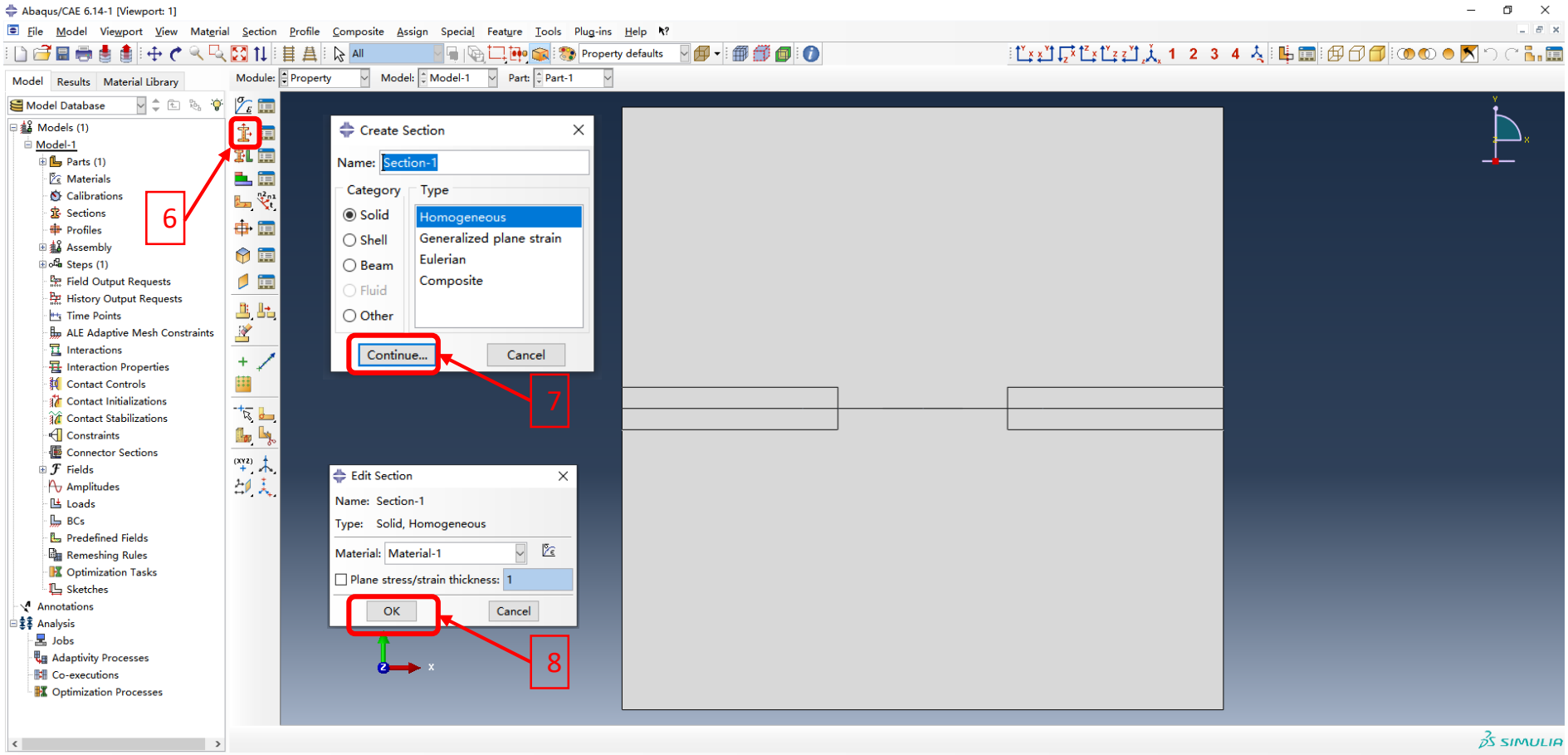
断裂相场方法模拟裂纹扩展

建模步骤（Property）



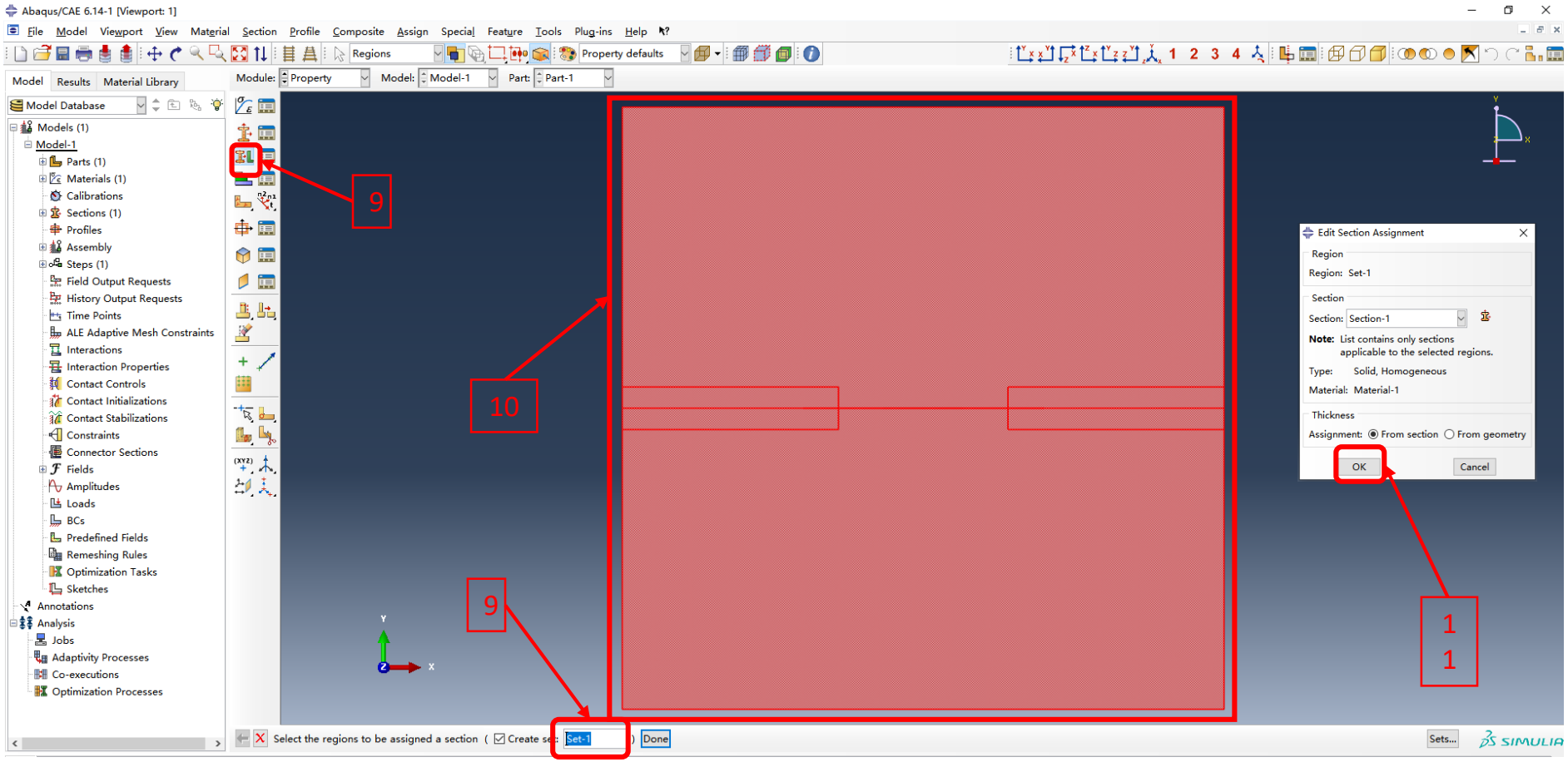
断裂相场方法模拟裂纹扩展

建模步骤（Property）



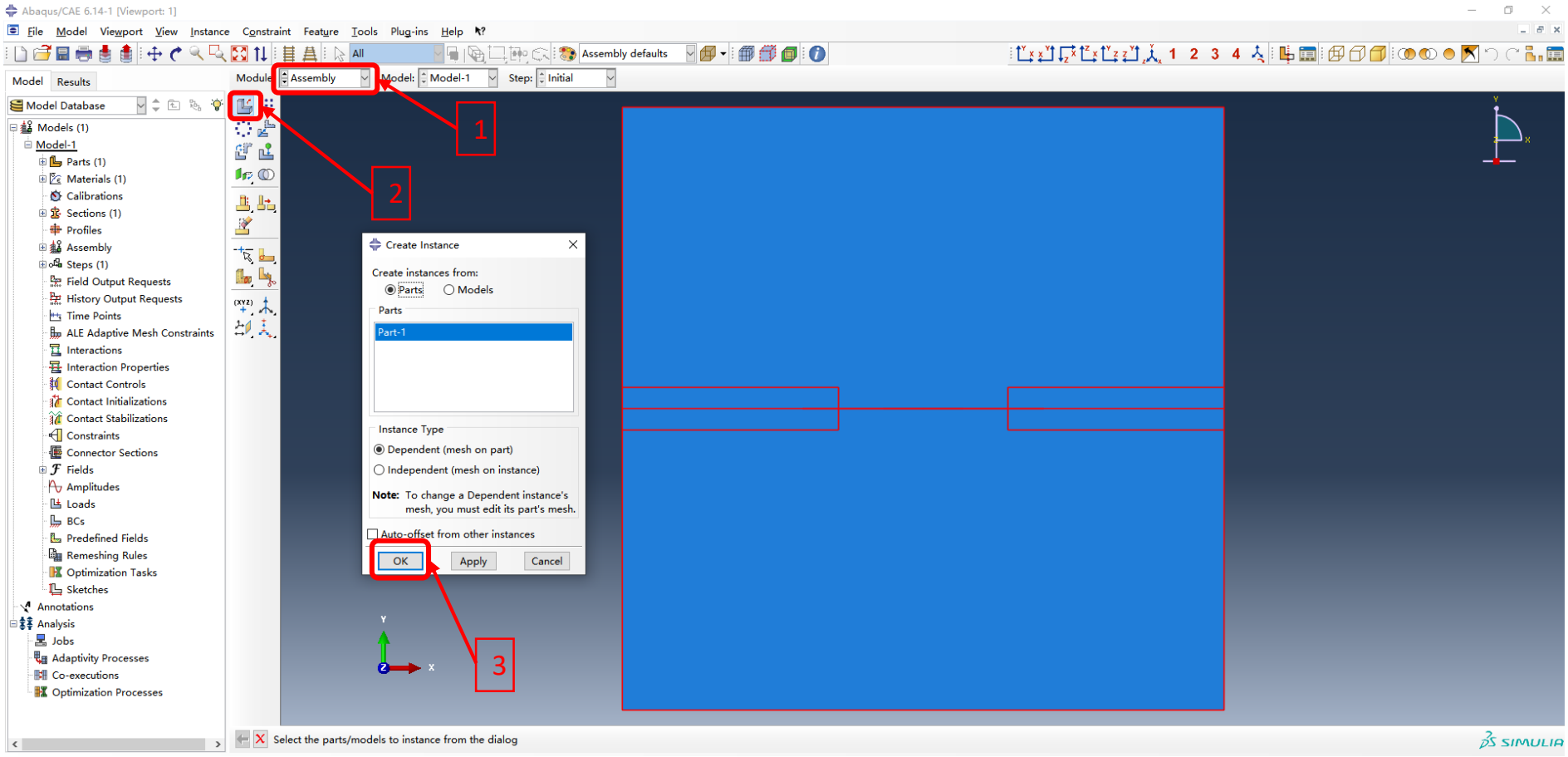
断裂相场方法模拟裂纹扩展

建模步骤（Property）



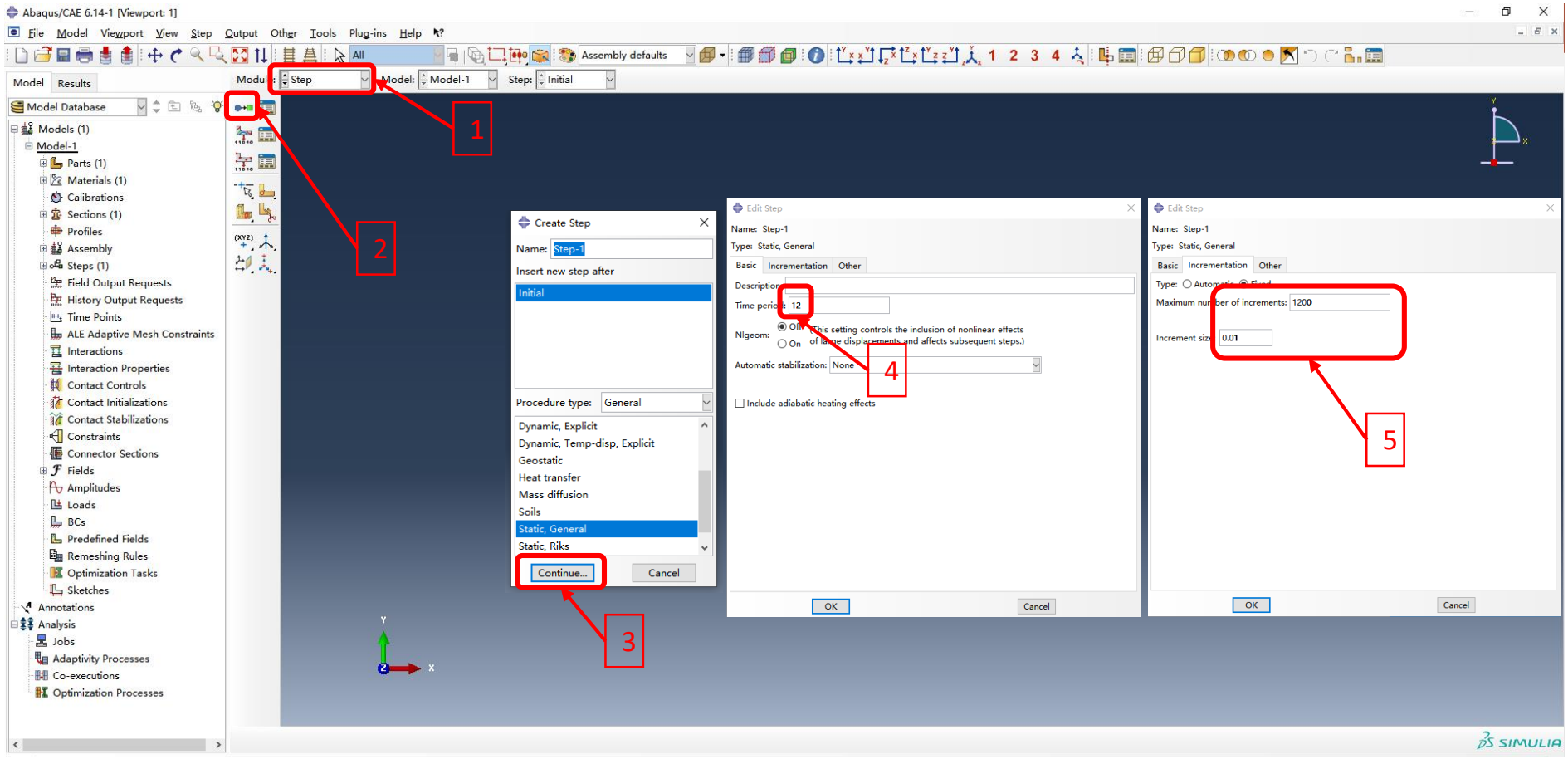
断裂相场方法模拟裂纹扩展

建模步骤（Assembly）



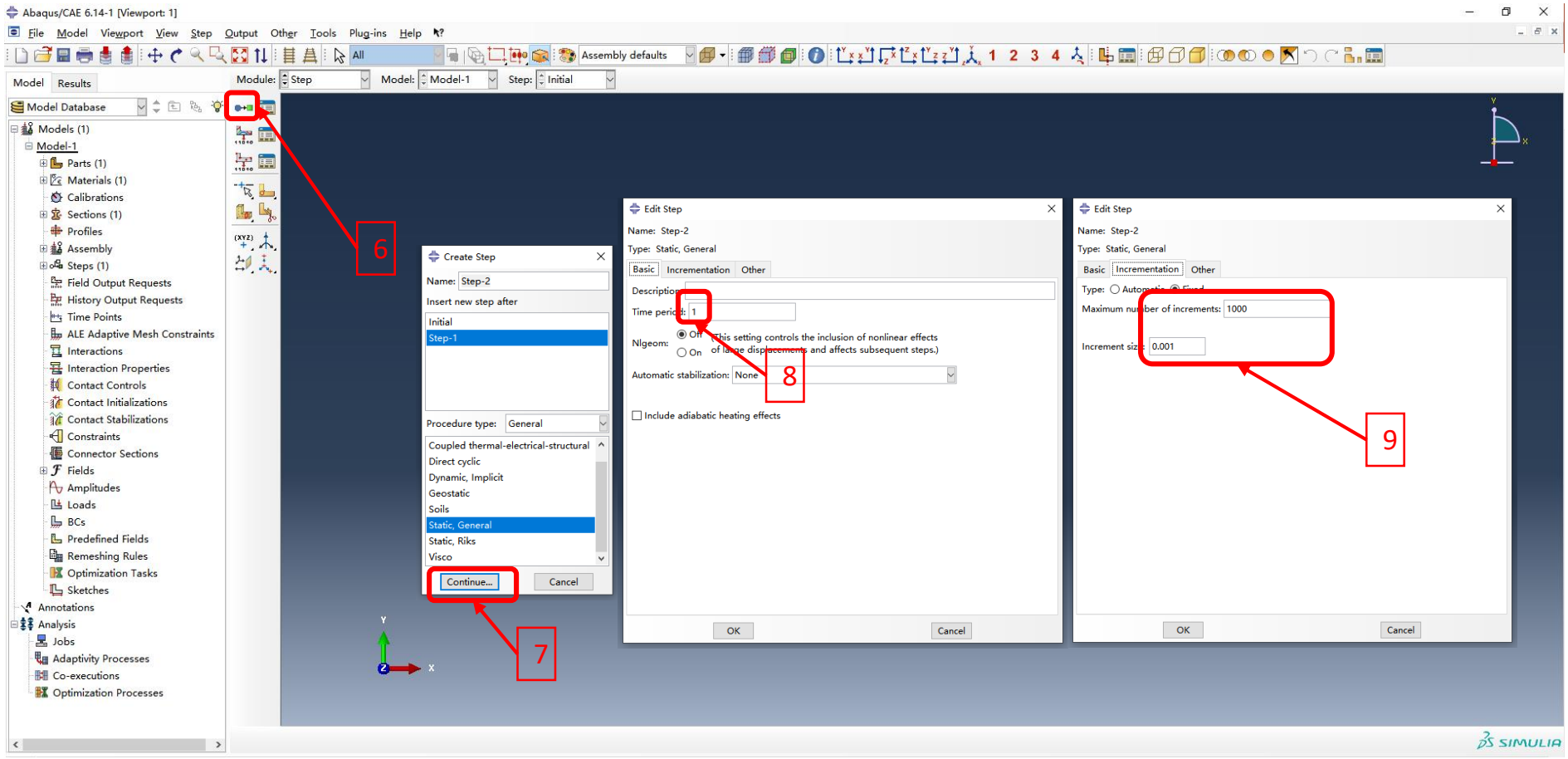
断裂相场方法模拟裂纹扩展

建模步骤（Step）



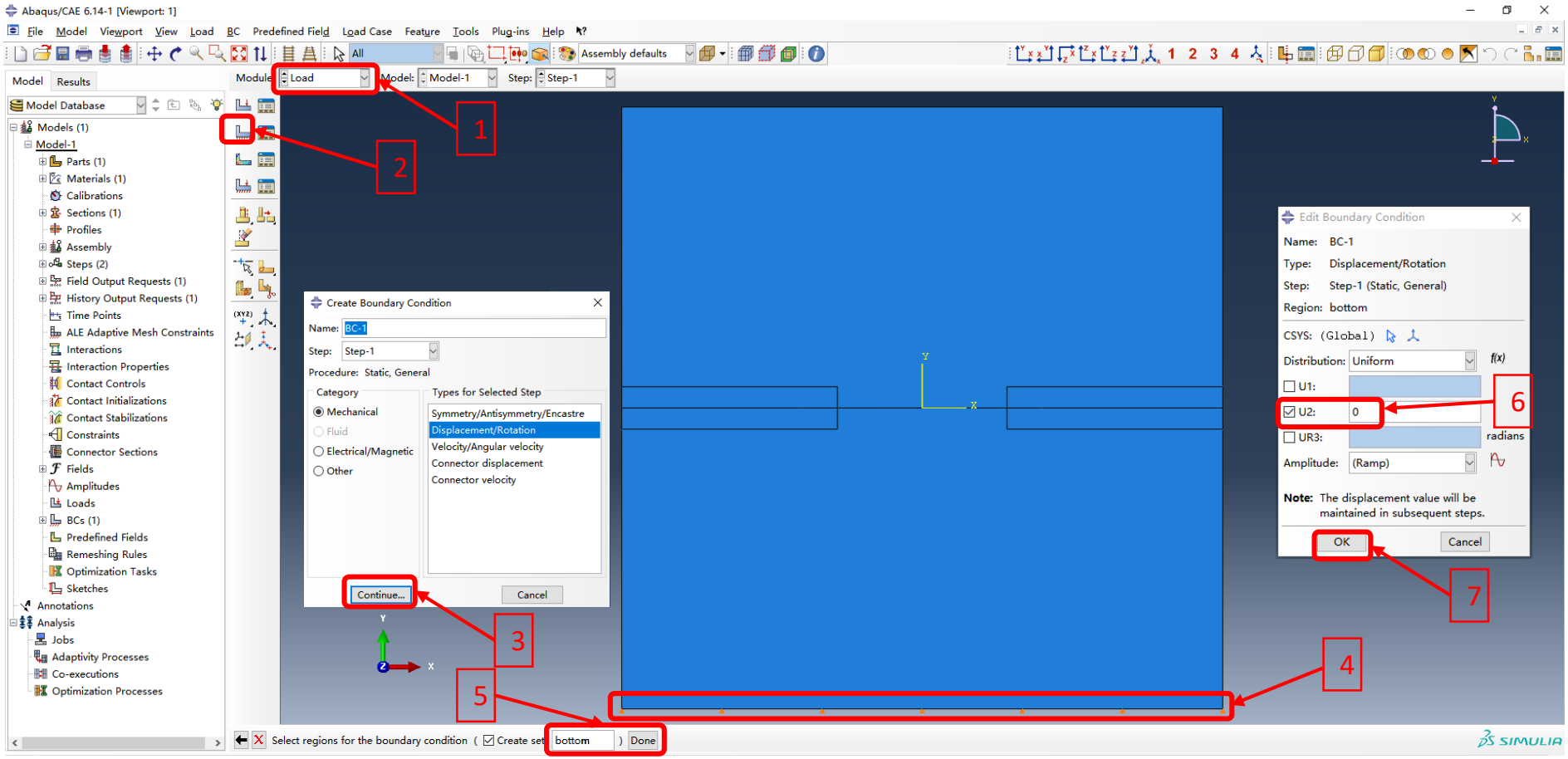
断裂相场方法模拟裂纹扩展

建模步骤（Step）



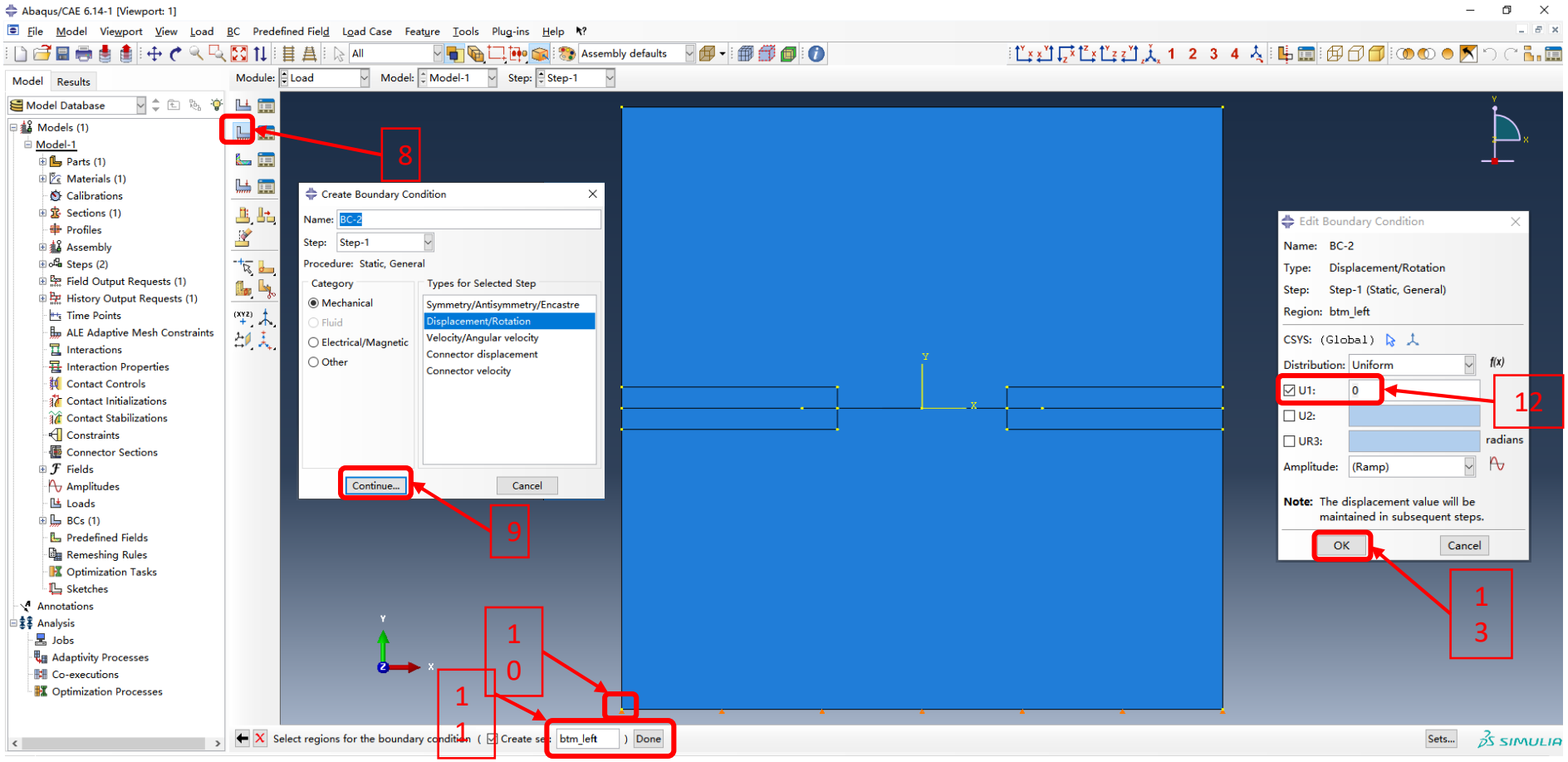
断裂相场方法模拟裂纹扩展

建模步骤（load）



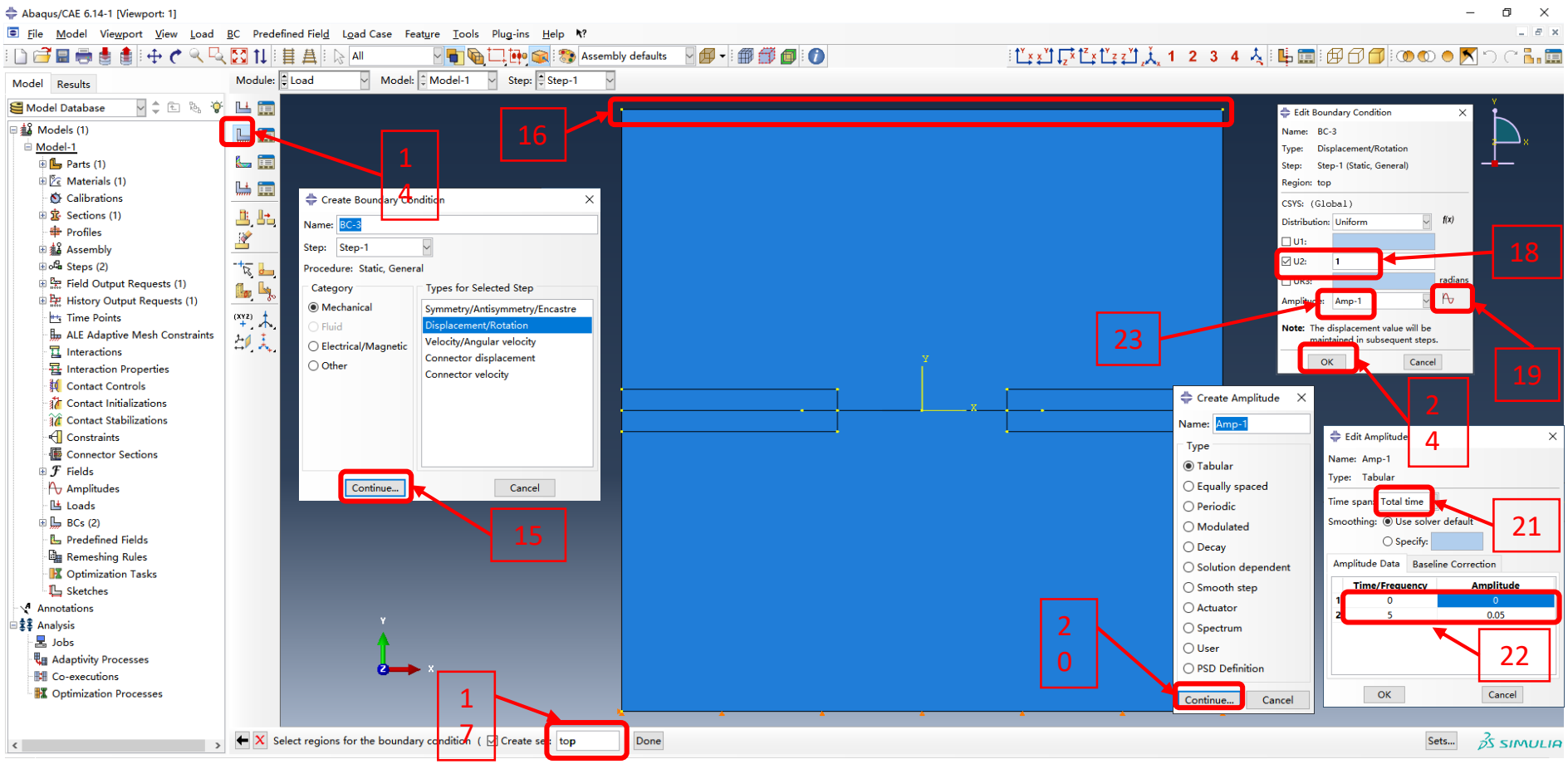
断裂相场方法模拟裂纹扩展

建模步骤（load）



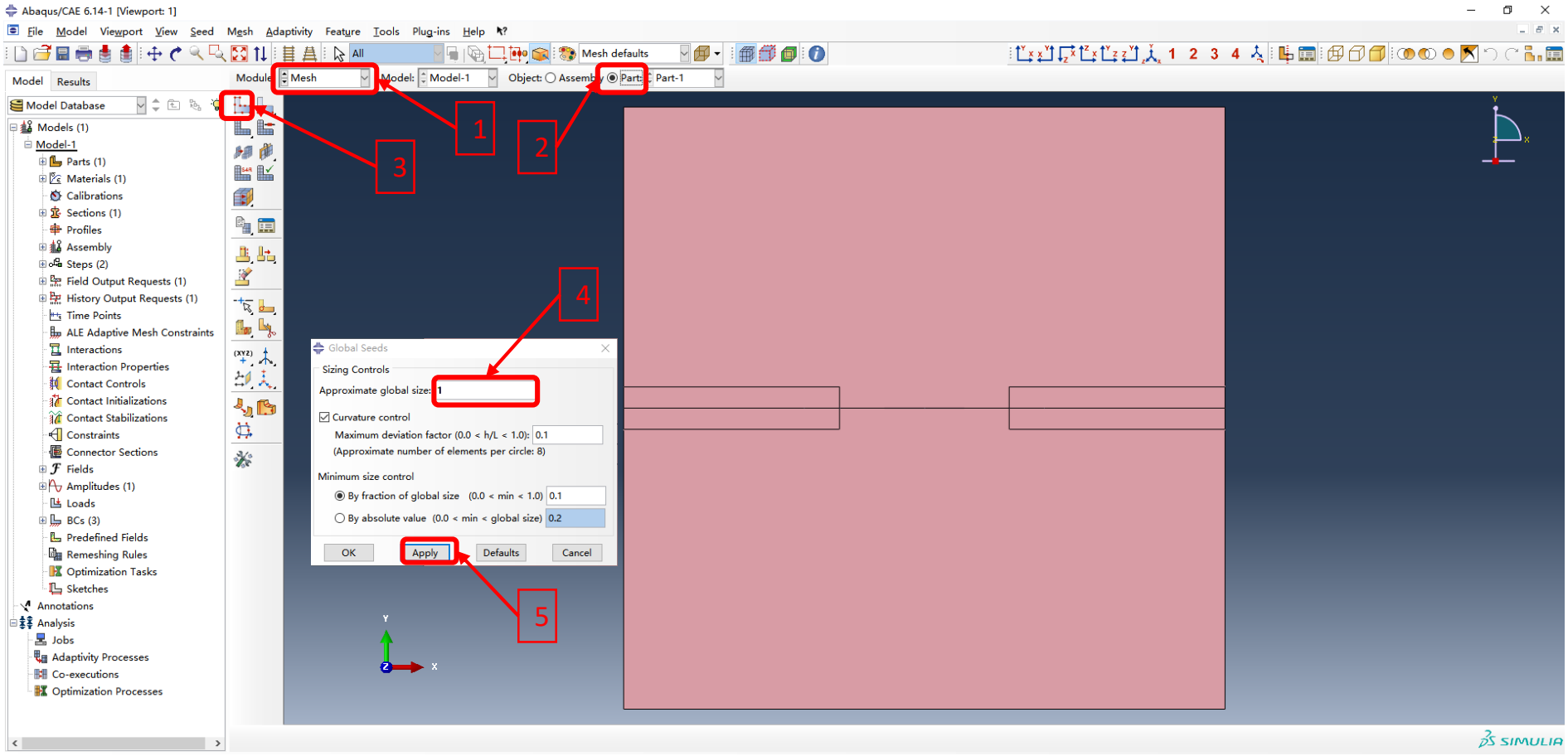
断裂相场方法模拟裂纹扩展

建模步骤（load）



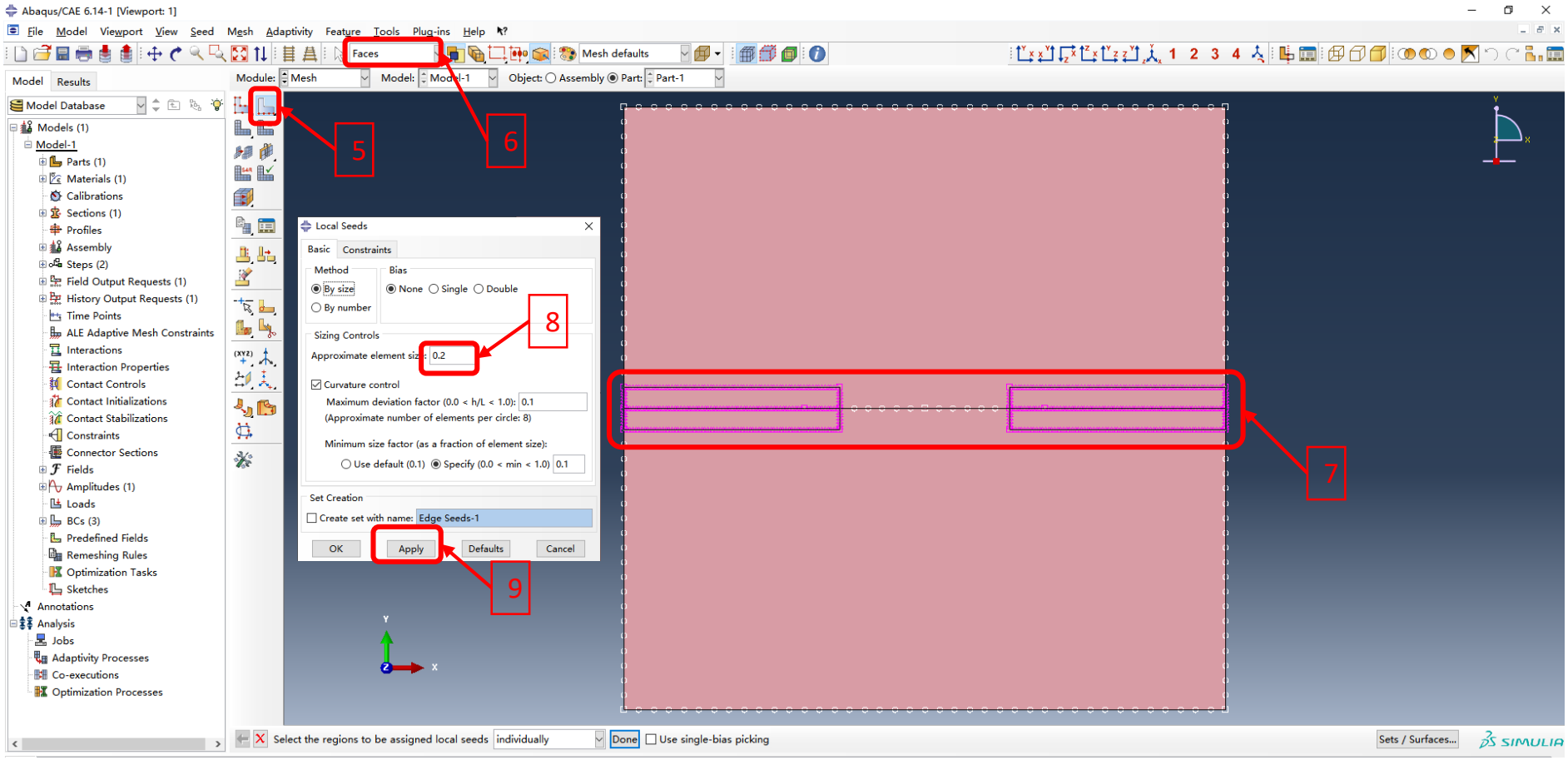
断裂相场方法模拟裂纹扩展

建模步骤（mesh）



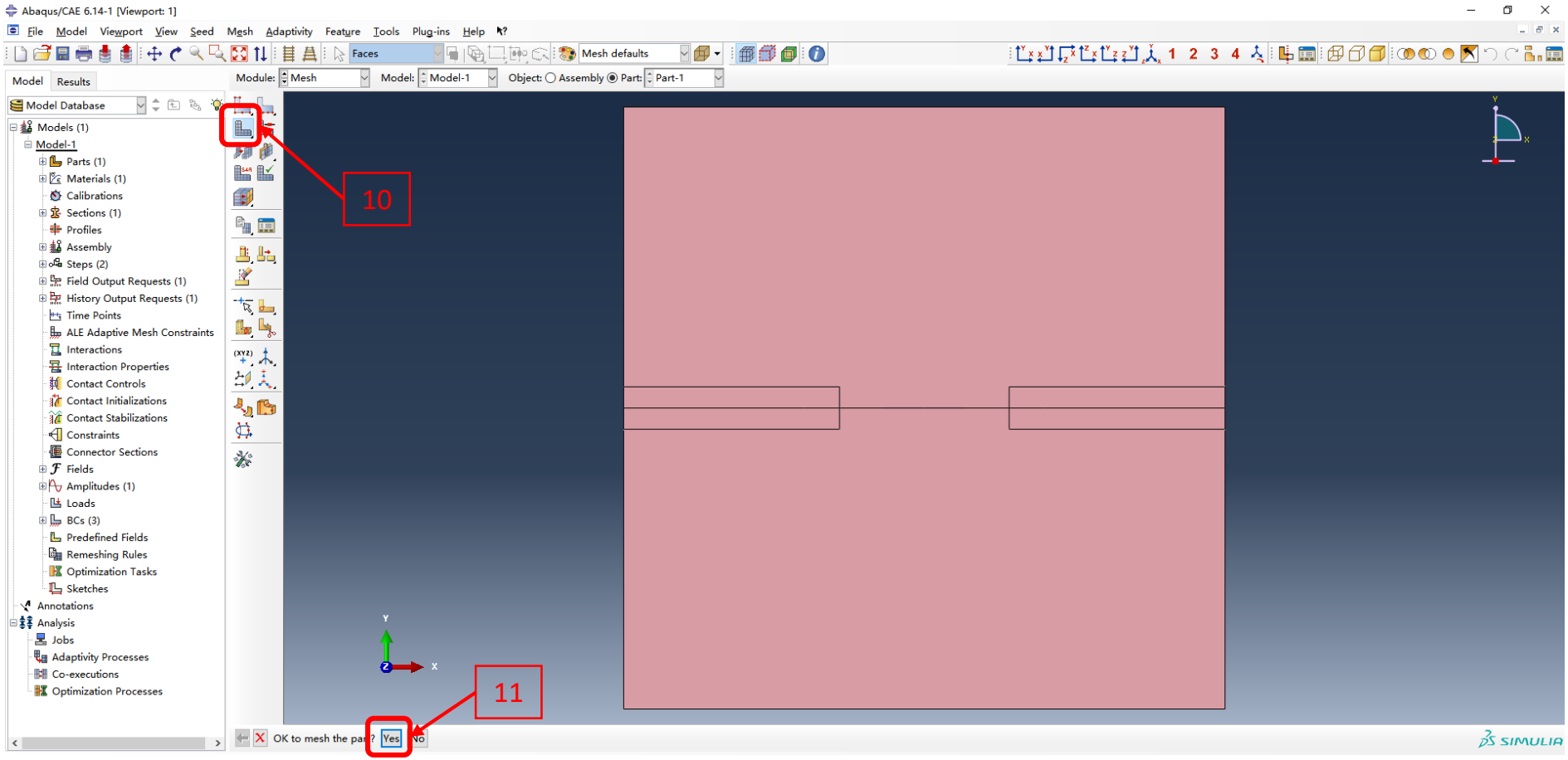
断裂相场方法模拟裂纹扩展

建模步骤（mesh）



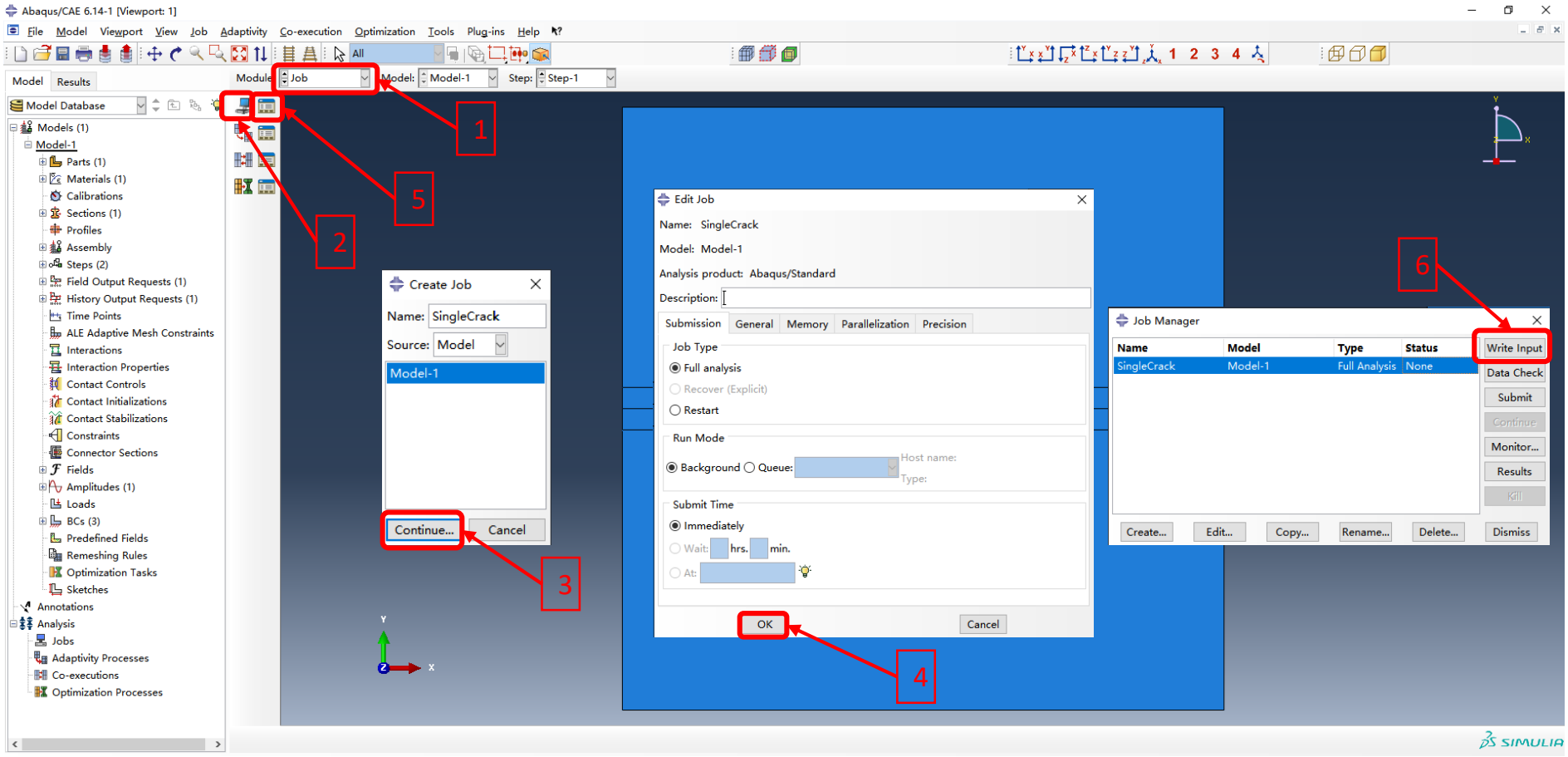
断裂相场方法模拟裂纹扩展

建模步骤（mesh）



断裂相场方法模拟裂纹扩展

建模步骤（job,生成inp文件）



断裂相场方法模拟裂纹扩展

修改inp文件和编写for文件

原始的inp文件

……

*Element, type=CPS4R
单元编号 单元节点编号
*Nset, nset=Set-1, generate
起始节点编号, 起始节点编号 , 1
*Elset, elset=Set-1, generate
起始单元编号, 起始单元编号 , 1

……

修改思想：得到代表裂纹场、位移场以及可视化的三层相同信息的单元

1.定义单元类型，复制三次单元信息分别分配给三个不同模块并重新编号

2.给不同模块的单元集合重命名

3.给不同模块的单元赋代入的参数信息

修改后的inp文件

……

*User element, nodes=4, type=U1, properties=3, coordinates=2, VARIABLES=8
3
*Element, type=U1
1,单元节点编号
……
n,单元节点编号
*Elset, elset=Set-1, generate
1, n, 1
*Uel property, elset=Set-1
0.1, 5e-3, 1.0

裂纹场单元

*User element, nodes=4, type=U2, properties=4, coordinates=2, VARIABLES=56
1,2
*Element, type=U2
n+1,单元节点编号
……
2n,单元节点编号
*Elset, elset=Set-1_U, generate
n+1, 2n, 1
*Uel property, elset=Set-1_U
210.0, 0.3, 1.0, 1.0e-7

位移场单元

*Element, TYPE=CPS4, elset=umatelem
2n+1,单元节点编号
……
3n,单元节点编号
*Solid Section, elset=umatelem, material=umat
1.0
*Elset, elset=umatelem, instance=Part-1-1, generate
2n+1, 3n, 1

可视化单元

*Nset, nset=Set-1, generate
起始节点编号, 起始节点编号 , 1
……

编写for文件

输入的参数信息：

Young's modulus E : 210 GPa

Poisson's ratio ν : 0.3

thickness of the element h : 1 mm

Stability parameter k : 1e-9

Length scale parameter l_0 0.4 mm

Fracture surface energy release rate g_c : 2.7e-3 kN/mm

For文件：UEL+UMAT

SingleCrack_UEL.inp
SingleCrack_UEL_PS.for

断裂相场方法模拟裂纹扩展

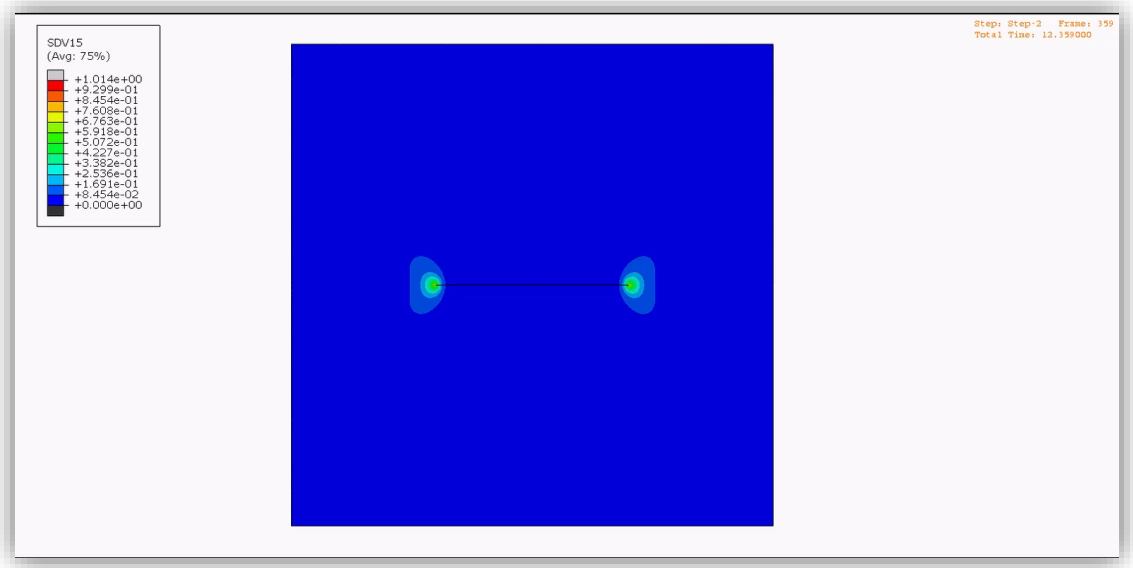
程序提交

```
cp ~/WORK/winterschool/day5/phase_field_lyy/case4/abaqus_run.sh ./
cp ~/WORK/winterschool/day5/phase_field_lyy/case4/SingleCrack_UEL.inp ./
cp ~/WORK/winterschool/day5/phase_field_lyy/case4/SingleCrack_UEL_PS.for ./
```

```
[train1@ln01 case4]$ ls
abaqus_run.sh  SingleCrack_UEL.inp  SingleCrack_UEL_PS.for
```

```
[train1@ln01 case4]$ sbatch abaqus_run.sh
Submitted batch job 119772
```

结果展示



Thank you for listening

陆宇阳

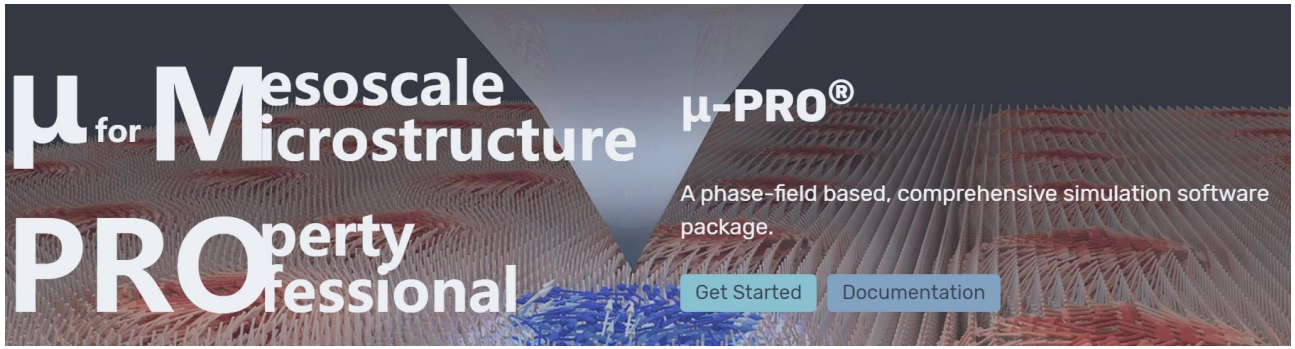
Email : luyuyang@mail.ustc.edu.cn

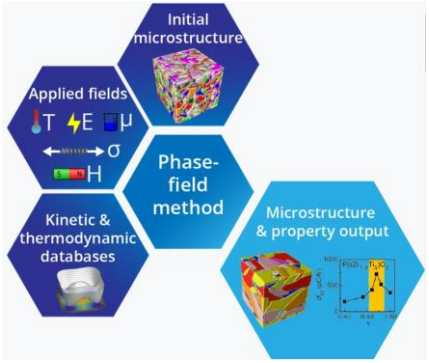
中国科学技术大学

University of Science and Technology of China



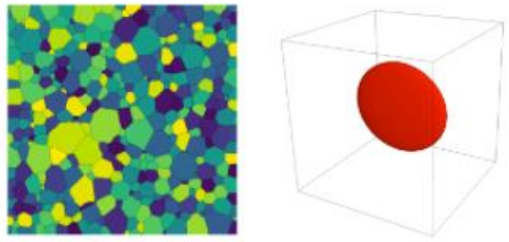

工具软件介绍





美国宾州州立大学陈龙庆教授团队开发的μ-PRO软件包http://mupro.co/

德国波鸿鲁尔大学的Igo Steinbach教授团队开发的OpenPhase Software （https://openphase-solutions.com/）



美国密歇根大学安娜堡分校团队开发的PRISMS-PF软件（prisms-center.github.io/phaseField/）

工具软件介绍

MOOSE

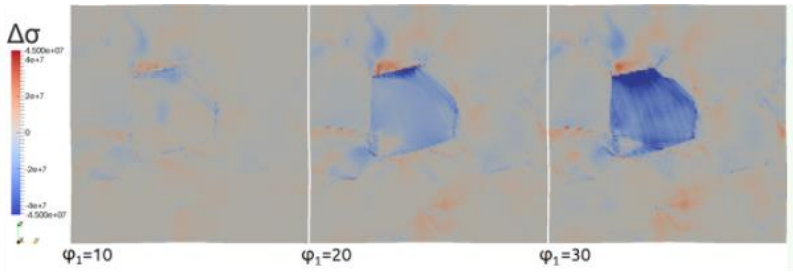
Multiphysics Object-Oriented Simulation Environment

An open-source, parallel finite element framework

https://mooseframework.org/ 美国INL国家实验室

DAMASK

Düsseldorf Advanced Material Simulation Kit



https://damask.mpie.de

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