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Phase-field modeling of solute precipitation / dissolution using MOOSE: A finite element method

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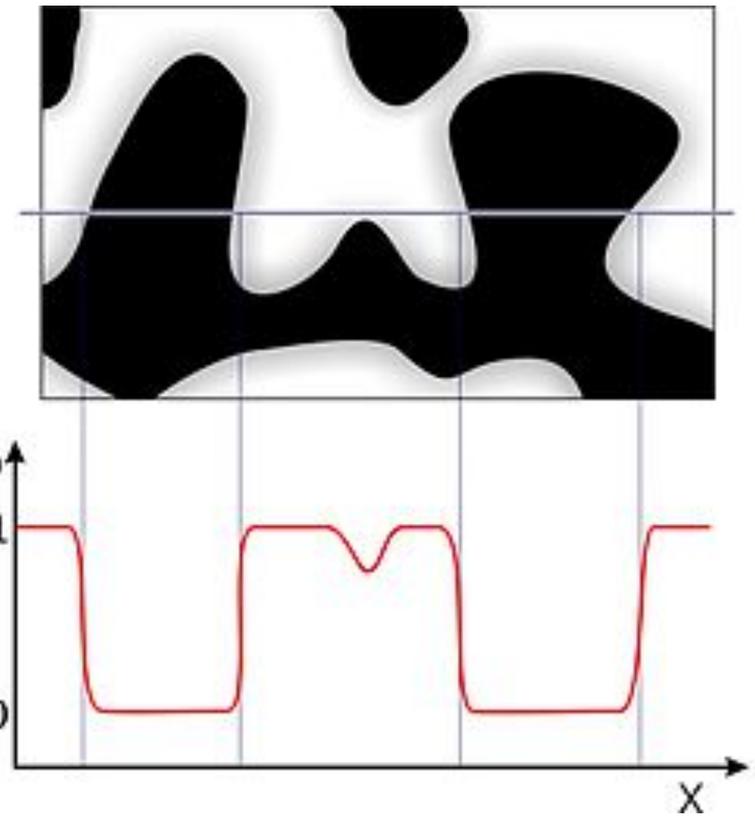
Phase field model

- Mathematical model for solving interfacial problems
- Two distinct values (-1 and +1) in each of the phases (solid and liquid)
- Free energy function

$$F = \int_{\Omega} [f_{loc}(\phi, c) + f_{grad}(\phi) + E_d] dV$$



- Gradient energy density (chemical potential)

$$\frac{\partial \phi}{\partial t} = -L \frac{\partial F}{\partial \phi}$$

- Gradient free energy function

$$f_{grad}(\phi) = \sum_{i}^{N} \frac{k_i}{2} |\nabla \phi|^2$$

- Local free energy function: a double well function

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Problem and Method

- Precipitation / Dissolution
- A (solid) <----------> A (liquid)

- Not real chemical reaction: A + B = C

- Finite element method (FEM) using MOOSE, a framework to solve partial differential equation (PDE) by Newton's method
- We only need to write down the weak form and jacobian of PDE, and implement the equations in code (C++)

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Equations

Governing equations:

$$\tau \frac{\partial \phi}{\partial t} = \varepsilon^2 \nabla^2 \phi - \left(\frac{\partial f_1}{\partial \phi} + \lambda c \frac{\partial f_2}{\partial \phi} \right) - \varepsilon^2 |\nabla \phi| \kappa$$

$$\frac{\partial c}{\partial t} = D \nabla^2 c + \frac{1}{2bk_c} \frac{\partial \phi}{\partial t} \left(1 + \frac{D \nabla^2 \phi - {}^{\partial \phi}/_{\partial t}}{k |\nabla \phi|}\right)$$

$c = \dfrac{C - C_e}{C_e}$, *Ce* is equlibrium concentration

Local energy funciton: $f_1 = -\frac{1}{2}\phi^2 + \frac{1}{4}\phi^4$

$$f_2 = \phi - \frac{1}{3}\phi^3$$

$$\tau = \alpha \lambda \frac{\varepsilon^2}{D} \left(\frac{5}{3} + \frac{\sqrt{2} D}{k \varepsilon} \right)$$

Xu and Meakin, 2008, Phase-field modeling of solute precipitation and dissolution, The Journal of Chemical Physics, 129, 014705.

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Equations

- Curvature

$$\kappa = \nabla \cdot \hat{n} = \nabla \cdot \frac{\nabla \phi}{|\nabla \phi|} = \frac{1}{|\nabla \phi|}\left[\nabla^2 \phi - \frac{\nabla \phi \, \nabla \cdot |\nabla \phi|}{|\nabla \phi|}\right]$$

- Weak Form

$$\left(\psi, \tau \frac{\partial \phi}{\partial t}\right) + (\nabla \psi, \varepsilon^2 \nabla \phi) - \langle \psi, \varepsilon^2 \nabla \phi \cdot \hat{n} \rangle + \left(\psi, \frac{\partial f_1}{\partial \phi} + \lambda c \frac{\partial f_2}{\partial \phi}\right) + (\psi, \varepsilon^2 |\nabla \phi| \kappa) = 0$$

$$\left(\psi, \frac{\partial c}{\partial t}\right) + (\nabla \psi, D \nabla c) - \langle \psi, D \nabla c \cdot \hat{n} \rangle - \left(\psi, \frac{1}{2bk_c} \frac{\partial \phi}{\partial t}\left(1 + \frac{D\nabla^2 \phi - {}^{\partial \phi}/_{\partial t}}{k|\nabla \phi|}\right)\right) = 0$$

Sun and Beckermann, 2007, Sharp interface tracking using the phase-field equation. Journal of Computational Physics, 220(2), 628-653.

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Dimensionless equations

$$\frac{\partial \phi}{\partial t} = \frac{1}{Pe'}\{\nabla^2\phi - (1-\phi^2)(\phi - \lambda c) - |\nabla\phi|\kappa'\}$$

$$\frac{\partial c}{\partial t} = \nabla^2 c + \alpha\frac{\partial \phi}{\partial t} + \alpha\frac{\nabla^2\phi - {}^{\partial\phi}/_{\partial t}}{Da|\nabla\phi|})$$

$$Pe' = \tau D/\varepsilon^2$$

$$\kappa' = \kappa\varepsilon$$

$$\lambda = Pe'/[\alpha(\frac{5}{3} + \sqrt{2}/Da)]$$

$$Pe = UL/D, Da = kL/D$$

Xu and Meakin, 2011. Phase-field modeling of two-dimensional solute precipitation/ dissolution: Solid finger and diffusion-limited precipitation, Journal of Chemical Physics, 134, 044137.

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Code framework

- include # C++ header file
- src # C++ source code file
  - base
  - Ics (initial conditions)
  - kernels
  - materials

```
ACAdd.C
ACAdd_dimensionless.C
ACGrad.C
ACGrad_dimensionless.C
ACLoc.C
ACLoc_dimensionless.C
ACTimeDerivative.C
ConcAdd.C
ConcAdd_dimensionless.C
ConcDiffusion.C
Convection.C
Diffusion.C
RandomNoise.C
RandomNoiseConc.C
TimeDerivative.C
```

```
Real
ACLoc::computeQpResidual()
{

  return - _test[_i][_qp] * (1 - _u[_qp]*_u[_qp]) * ( _u[_qp] - _lambda[_qp] * _c[_qp] ) ;

}

Real
ACLoc::computeQpJacobian()
{

  return - _test[_i][_qp] * _phi[_j][_qp] * ( 1 - 3 * _u[_qp]*_u[_qp]  + 2 * _lambda[_qp] * _c[_qp] * _u[_qp]);


}
```

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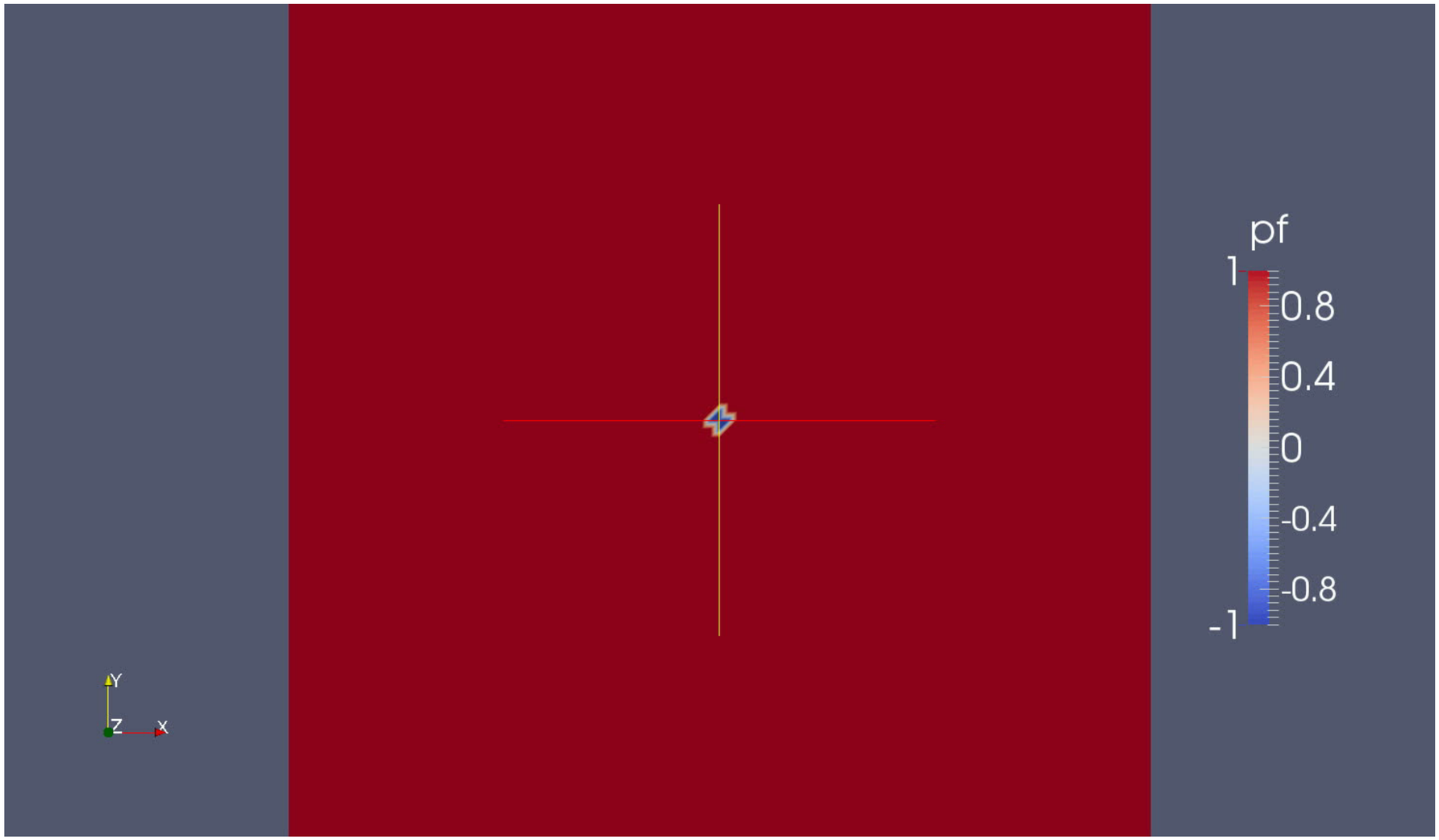
Dendrite growth (reaction-limited case)

- Damkohler number ≈ 1 (low reaction rate relatively to diffusion)

- Mesh: 50 × 50
- Domain: 10.0 × 10.0
- Reaction rate: 5.0
- Diffusion coef: 0.5
- Epsilon: 0.05

- dt = 0.005
- Timestep = 200



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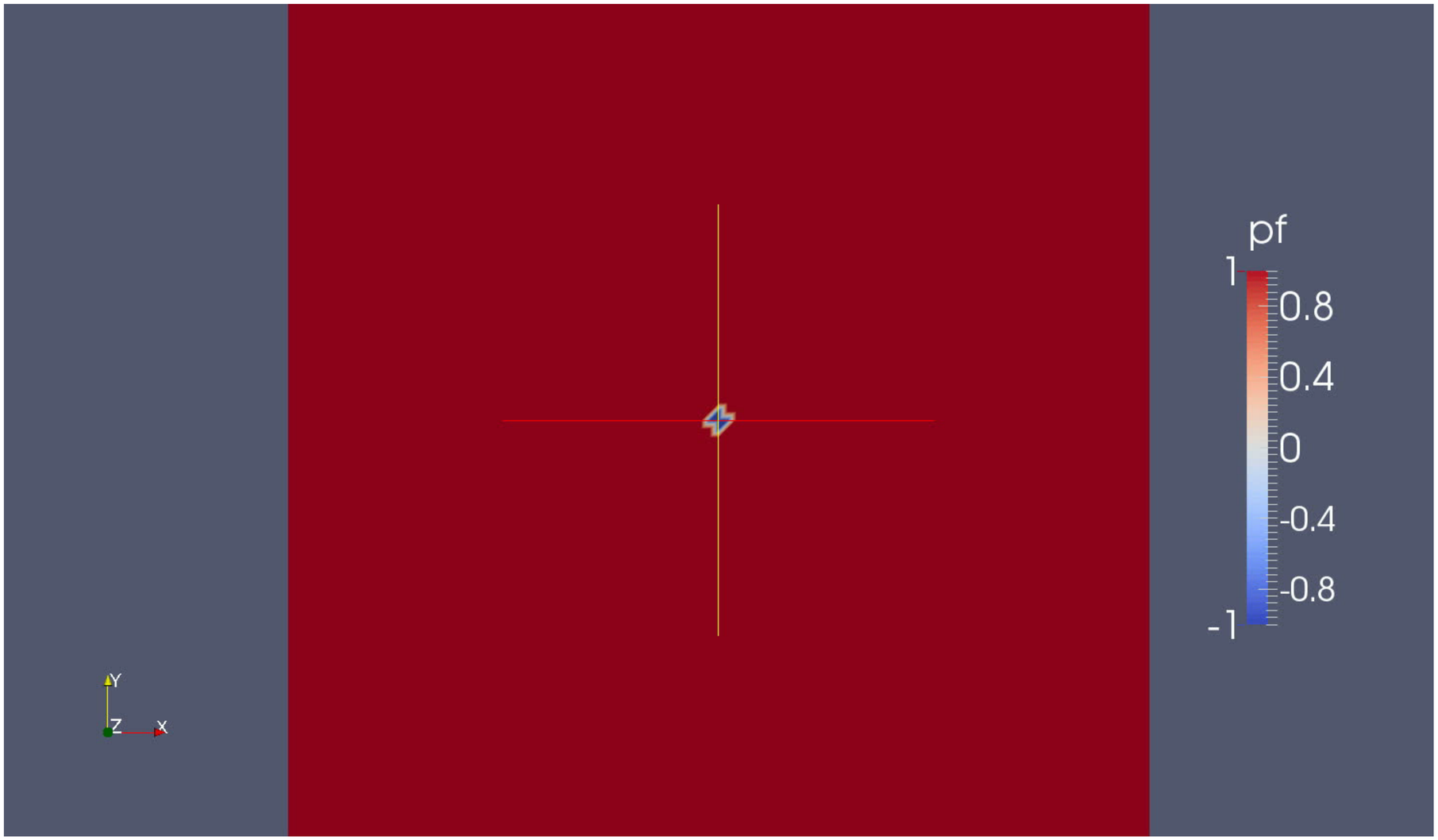
Dendrite growth (diffusion-limited case)

- Damkohler number ≈ 50,000

- dt = 0.01
- Timestep = 80



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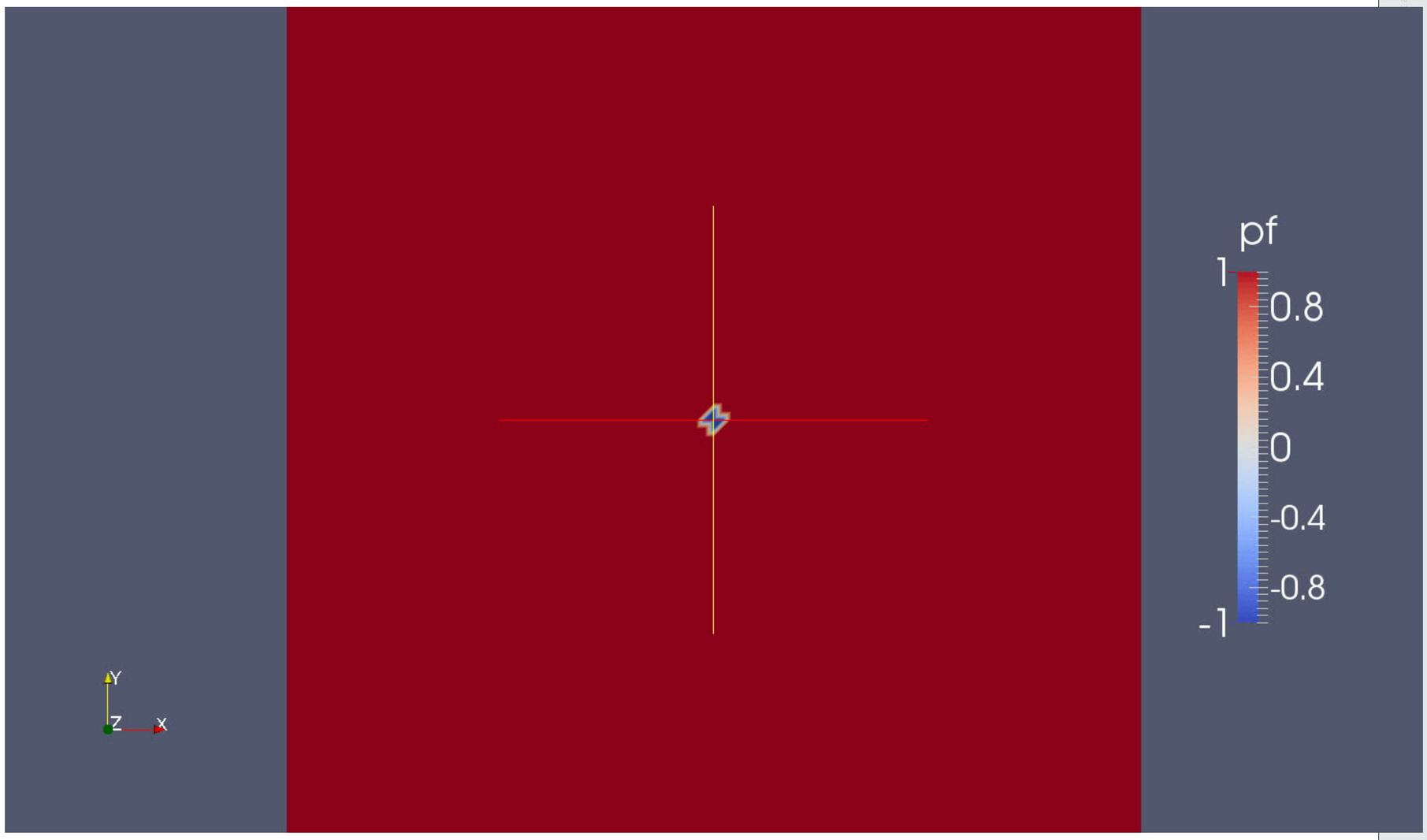
Dendrite growth (sidebranch)

- Damkohler number > 10,000
- Random noise was introduced

  $\alpha n(1-\phi)^2(1+\phi)^2$
- α is the amplitude of noise
- n is random number
- dt = 0.01
- Timestep = 80



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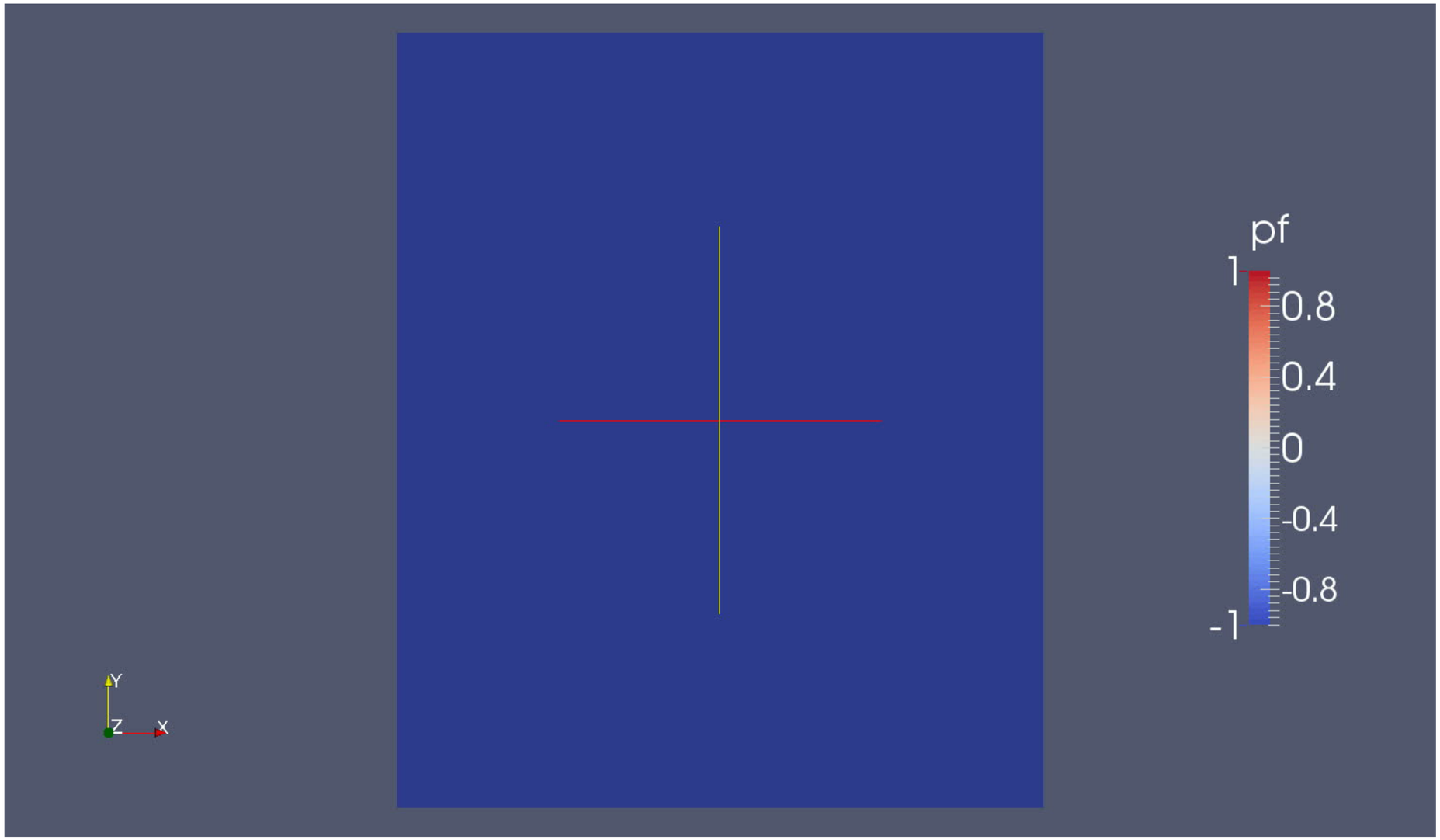
Dissolution

- All parameters are the same as sidebranch case with random noise



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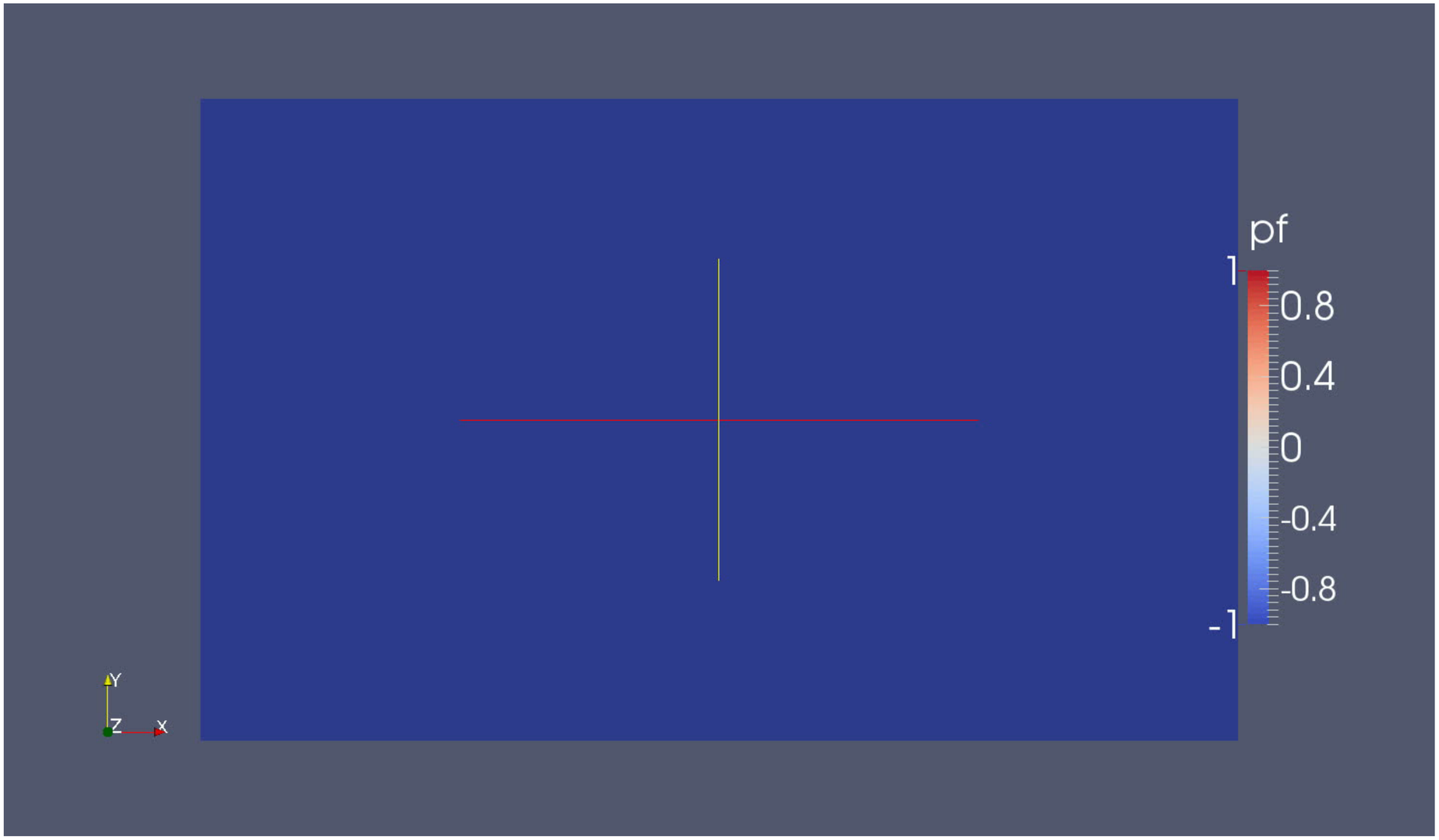
Dissolution (point source)

- Dissolution progress is slow

- dt = 0.01
- Timestep = 100



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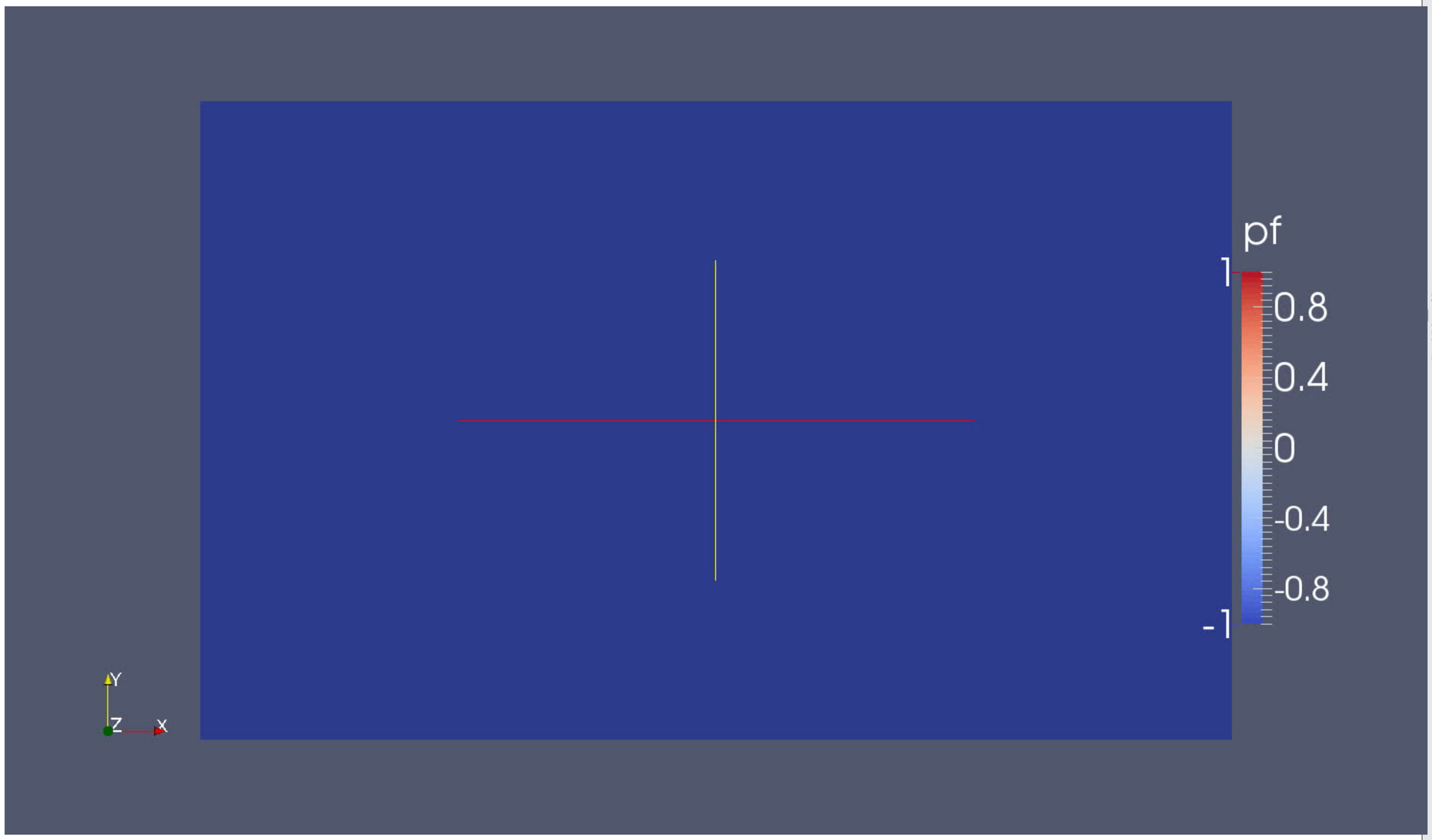
Dissolution (point source, with convenction)

- All parameters are same, except add a convenction term along x axis



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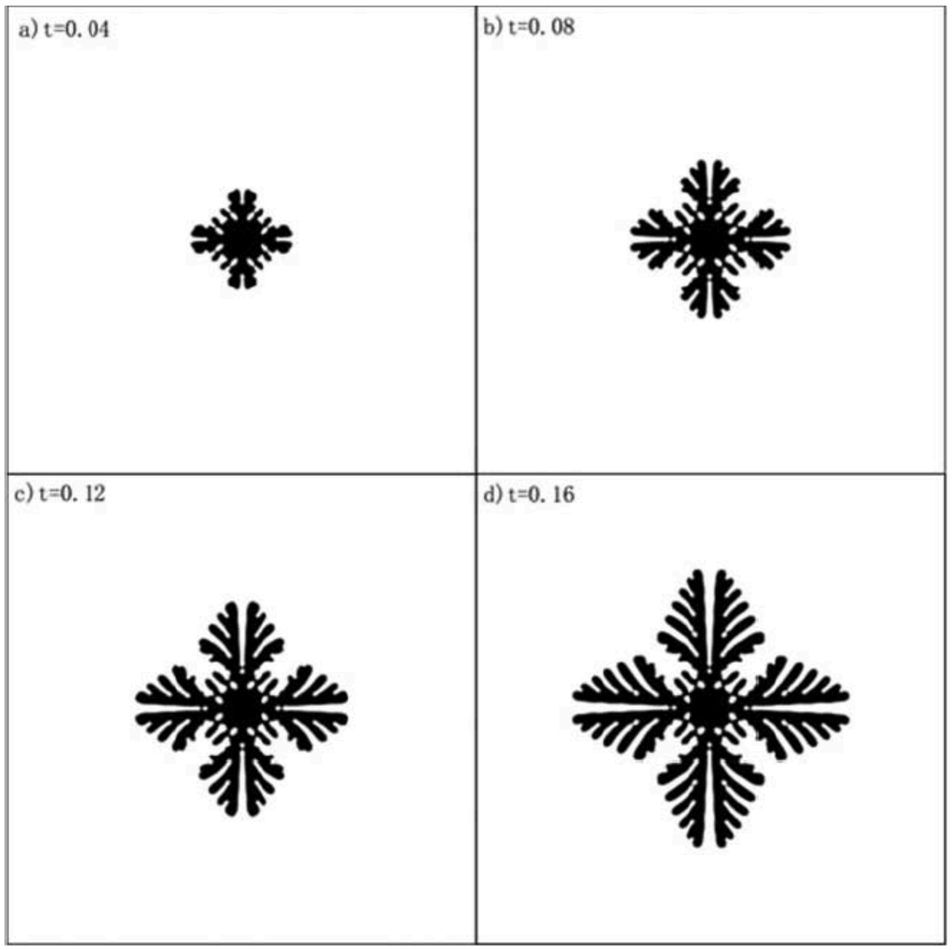
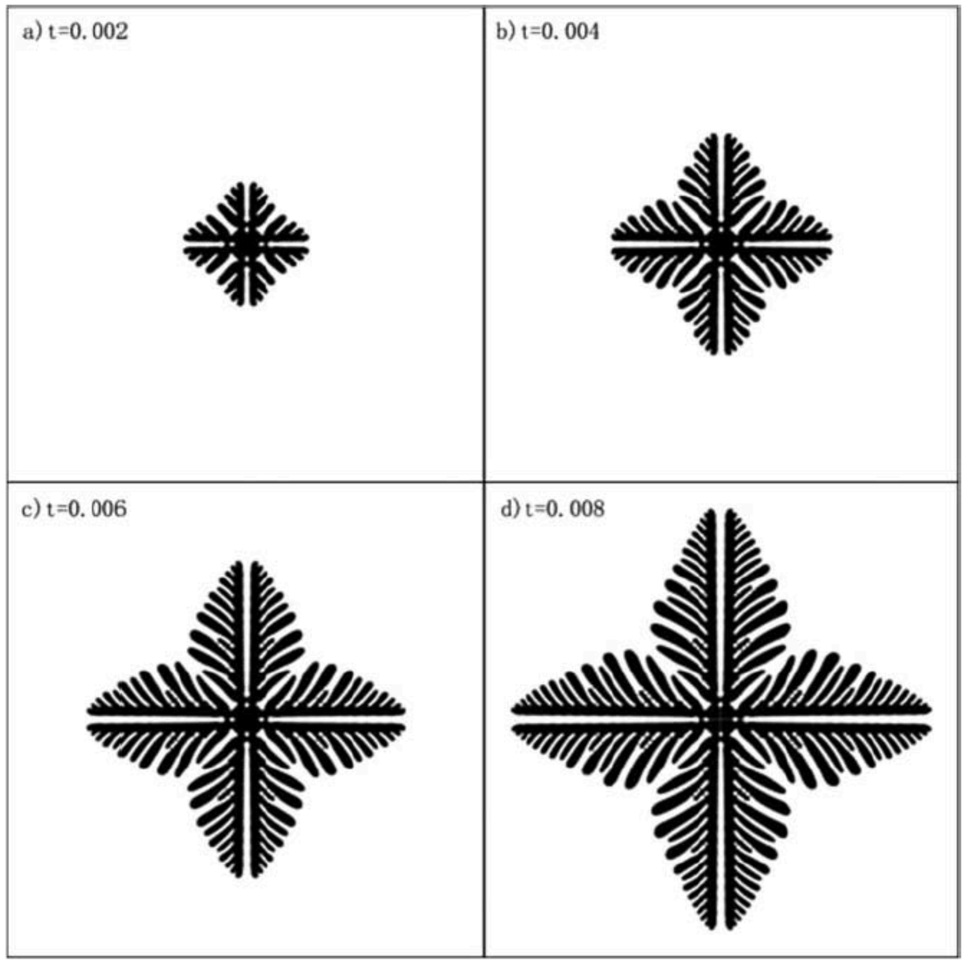
Something needs to improve

- Solid finger effect (diffuesd-limited case)





- We still cannot do that!

Xu and Meakin, 2011. Phase-field modeling of two-dimensional solute precipitation/ dissolution: Solid finger and diffusion-limited precipitation, Journal of Chemical Physics, 134, 044137.

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Possible reasons

- Different methods: finite element & finite difference
- Anisotropic： random noise
- Curvature expression
- Parameters chosen
- Code implementation
-

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What's next?

- Phase field model with chemical reaction
- A + B = C

- Explore new governing equations

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