NS Cahn-Hilliard description

$$\rho\frac{D\mathbf{u}}{Dt} = -\nabla p + \mu\nabla^2\mathbf{u} + \phi\nabla C$$

$$\nabla\cdot\mathbf{u} = 0$$

$$\frac{DC}{Dt} = \kappa\nabla^2\phi$$

$$\phi = \frac{\sigma}{\varepsilon}f'(C) - \sigma\varepsilon\nabla^2 C$$

Standard choice

$f(C) = (1-C)^2(1+C)^2/4$

$g(C) = (2+3C-C^3)/4$

Wetting boundary condition

$$\varepsilon\mu_f\frac{\partial C}{\partial t} = -\sigma\varepsilon\nabla C\cdot\boldsymbol{n} + (\gamma_1-\gamma_0)g'(C)$$

$$\mathbf{u}_s = 0$$

Solve for: $\mathbf{u}$, p, C

Parameters:

μ_f, ρ, μ, γ ($= \sigma\frac{2\sqrt{2}}{3}$ =surface tension)

$(\gamma_1-\gamma_0)/\gamma = \cos\theta_e$

ε, κ: interface width, mobility – treat as numerical parameters

NS Cahn-Hilliard description

$$\frac{D\mathbf{u}}{Dt} = -\nabla p + \frac{1}{Re}\nabla^2\mathbf{u} + \frac{1}{We}\phi\nabla C$$

$$\nabla \cdot \mathbf{u} = 0$$

$$\frac{DC}{Dt} = \frac{1}{Pe}\nabla^2\phi$$

$$\phi = f'(C) - Cn^2\nabla^2 C$$

Standard choice

$f(C) = (1-C)^2(1+C)^2/4$

$g(C) = (2 + 3C - C^3)/4$

Wetting boundary condition

$$Ca_f Cn \frac{\partial C}{\partial t} = -\frac{3}{2\sqrt{2}} Cn\, \nabla C \cdot \boldsymbol{n} + cos\theta_e g'(C)$$

$$\mathbf{u}_s = 0$$

Solve for: $\mathbf{u}$, p, C

Parameters:

Re, We, Pe, Ca_f, Cn

$$\frac{DC}{Dt} = \kappa \nabla^2 \phi$$
$$\phi = \frac{\sigma}{\varepsilon} f'(C) - \sigma\varepsilon\nabla^2 C$$

Standard choice
$$f(C) = (1-C)^2(1+C)^2/4$$
$$g(C) = (2+3C-C^3)/4$$

A two component mixture

Chemical potential phi may seem a bit mystical

But

Away from the interface, where C≈+-1:

C=1+c,   c<<1

Eqns become:

$$\frac{Dc}{Dt} = 2\alpha\nabla^2 c$$

Regular Fickian mass diffusion

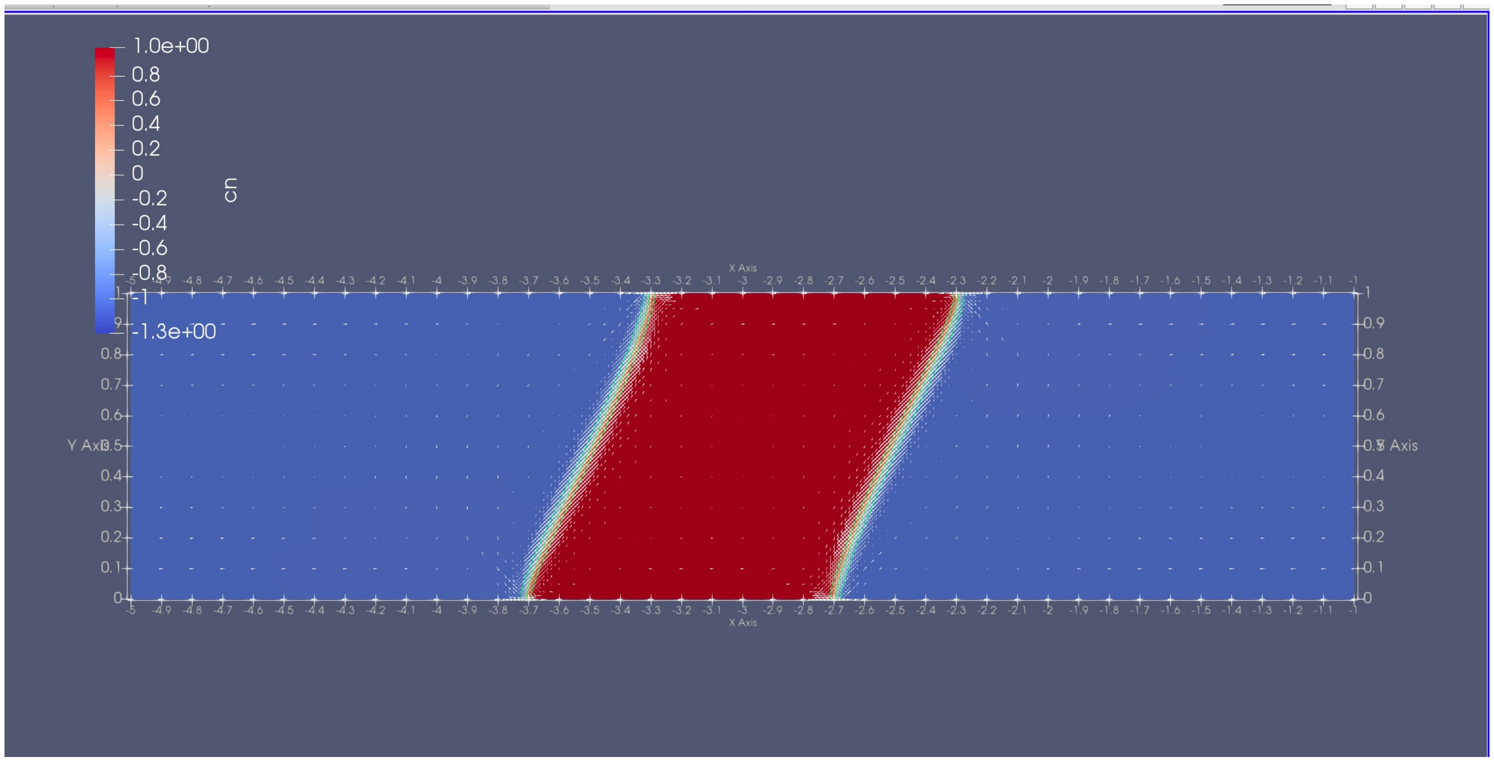
$$\alpha = \frac{3}{2\sqrt{2}}\frac{\kappa\gamma}{\varepsilon}$$

```
#### GENERAL INFORMATION ####
P100_cn01/out            < outplotfile
empty              < plotfiles/tmpSave1          < infile
1E-11          < GMRES-tolerance
1E-11          < CG-tolerance
5000           < max of loop in cg
0.004          < dt
30             < endtime
0.1            < time to print out information
0.1         < time to save results to disk
0.02           < time to check stop flag (define in femlego.stop)
0              < time limit (minute: 0=nolimit)
#### ADAPTIVE INFORMATION ####
0.0001                                   < errLow
0.0004           < errHi
0.002            < adaptHmin
0.001        < adaptive time
#### USER's PARAMETERS ####
3.978            < Reno
0.01           < Cahn
1.06           < Ca
100.0            < Pe
0.0          <Bo
0.0      < cos_theta
0.010            < eps_p
0.0            < eps_phi
0.0            < eps_c
1.040            < rad
0.01           < xi
100.0            < errfcn
0.99           < a
0.01          < rhom
0.01          < vism
0.0            < ksmt
1.0            < coupl
10.            < errcrf1
1000.0           < errcrf2
0.3                                       < dr
0.05          <ui    use as wall speed
0.0                                        <A
1000           < fric, controls slip
0.0            < lnk
0.0            <muf
```

/Users/gustava2/prog/paradapt-2.4/Couette_wetting/P100_cn01

Wall speed = +- 0.05

Ca= 1.06*0.02=0.053



```
#### GENERAL INFORMATION ####
P100_cn01/out            < outplotfile
empty            < plotfiles/tmpSave1            < infile
1E-11            < GMRES-tolerance
1E-11            < CG-tolerance
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0.0              < eps_phi
0.0              < eps_c
1.040            < rad
0.01             < xi
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0.01             < rhom
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1000.0           < errcrf2
0.3                                     < dr
0.05             <ui    use as wall speed
0.0                                     <A
1000             < fric, controls slip
0.0              < lnk
0.0              <muf
```
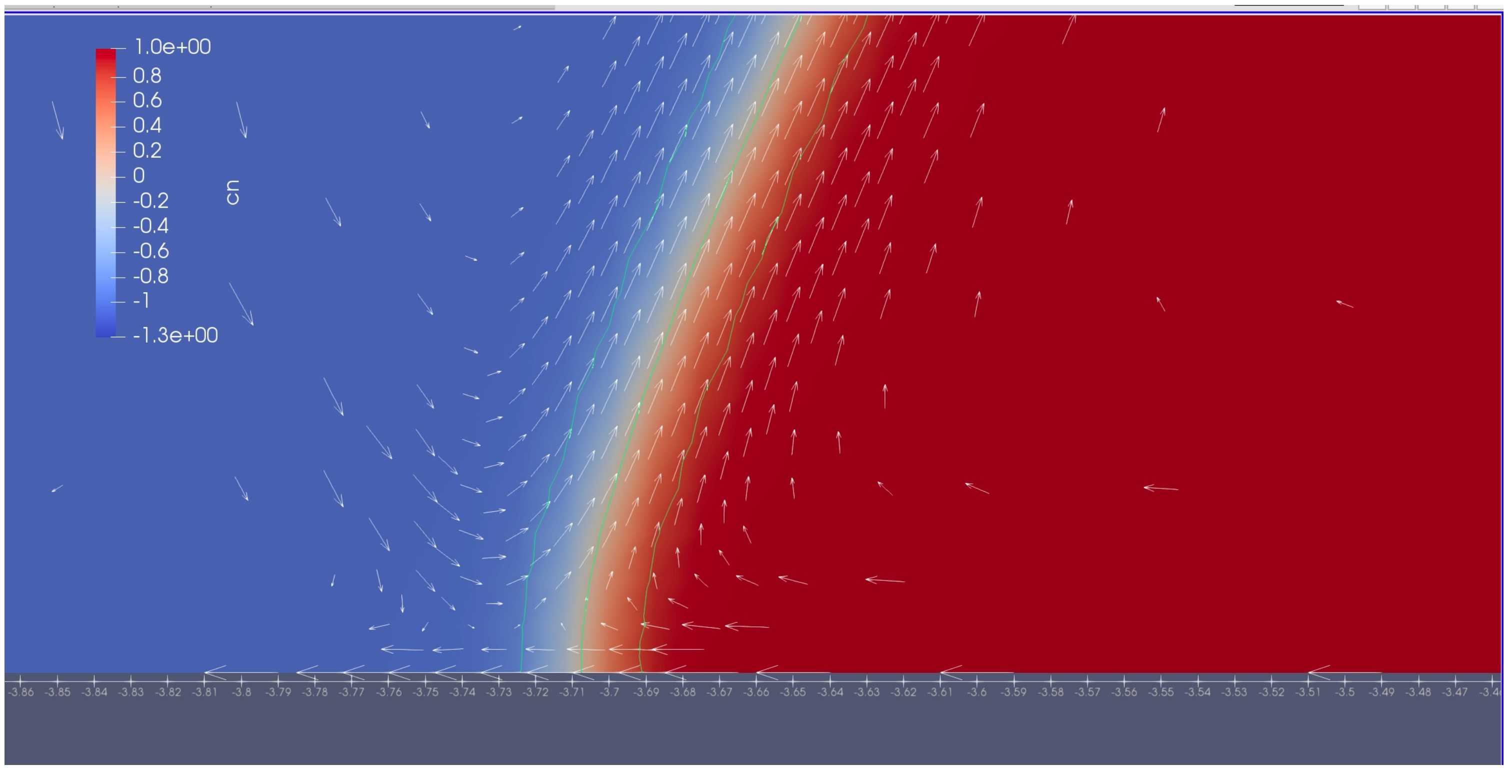

/Users/gustava2/prog/paradapt-2.4/Couette_wetting/P100_cn01

Wall speed = +- 0.05

Ca= 1.06*0.02=0.053



```
#### GENERAL INFORMATION ####
P100_cn01/out           < outplotfile
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0.0         <Bo
0.0       < cos_theta
0.010          < eps_p
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0.0          < eps_c
1.040          < rad
0.01          < xi
100.0           < errfcn
0.99          < a
0.01          < rhom
0.01          < vism
0.0          < ksmt
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10.          < errcrf1
1000.0          < errcrf2
0.3                                 < dr
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0.0                                   <A
1000          < fric, controls slip
0.0          < lnk
0.0          <muf
```
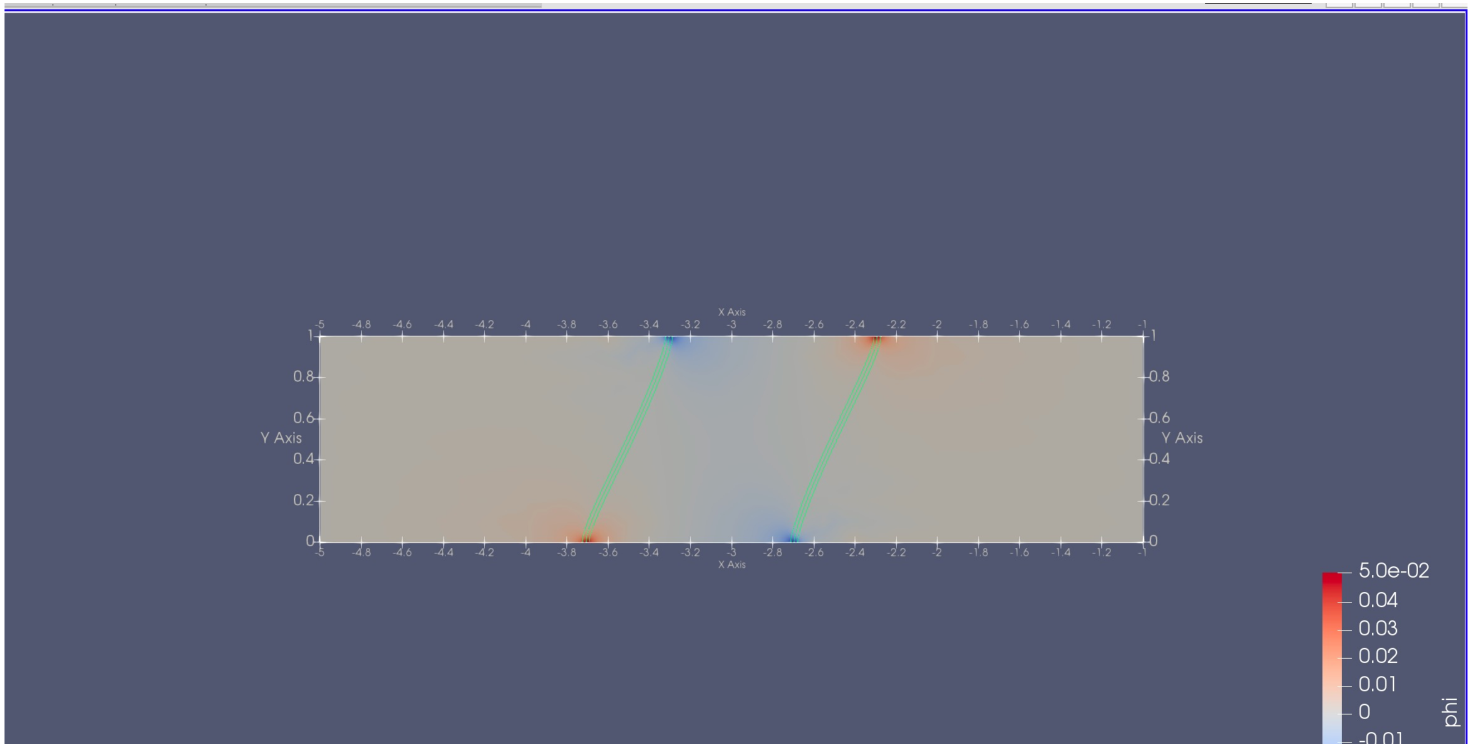

/Users/gustava2/prog/paradapt-2.4/Couette_wetting/P100_cn01

Wall speed = +- 0.05

Ca= 1.06*0.02=0.053



```
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0.0          < eps_c
1.040          < rad
0.01          < xi
100.0          < errfcn
0.99          < a
0.01         < rhom
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```
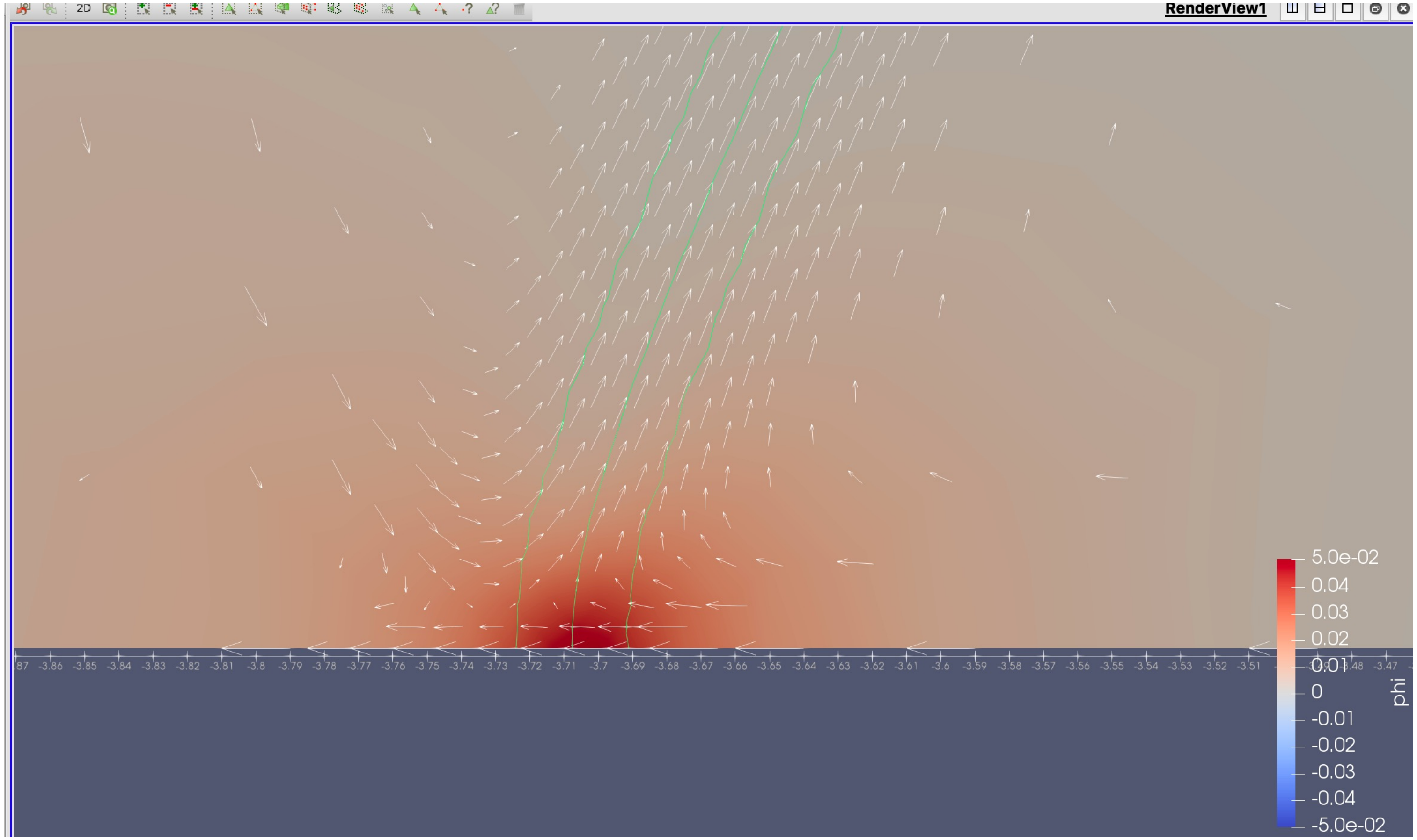

/Users/gustava2/prog/paradapt-2.4/Couette_wetting/P100_cn01

Wall speed = +- 0.05

Ca= 1.06*0.02=0.053



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0.01         < rhom
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0.0          <muf
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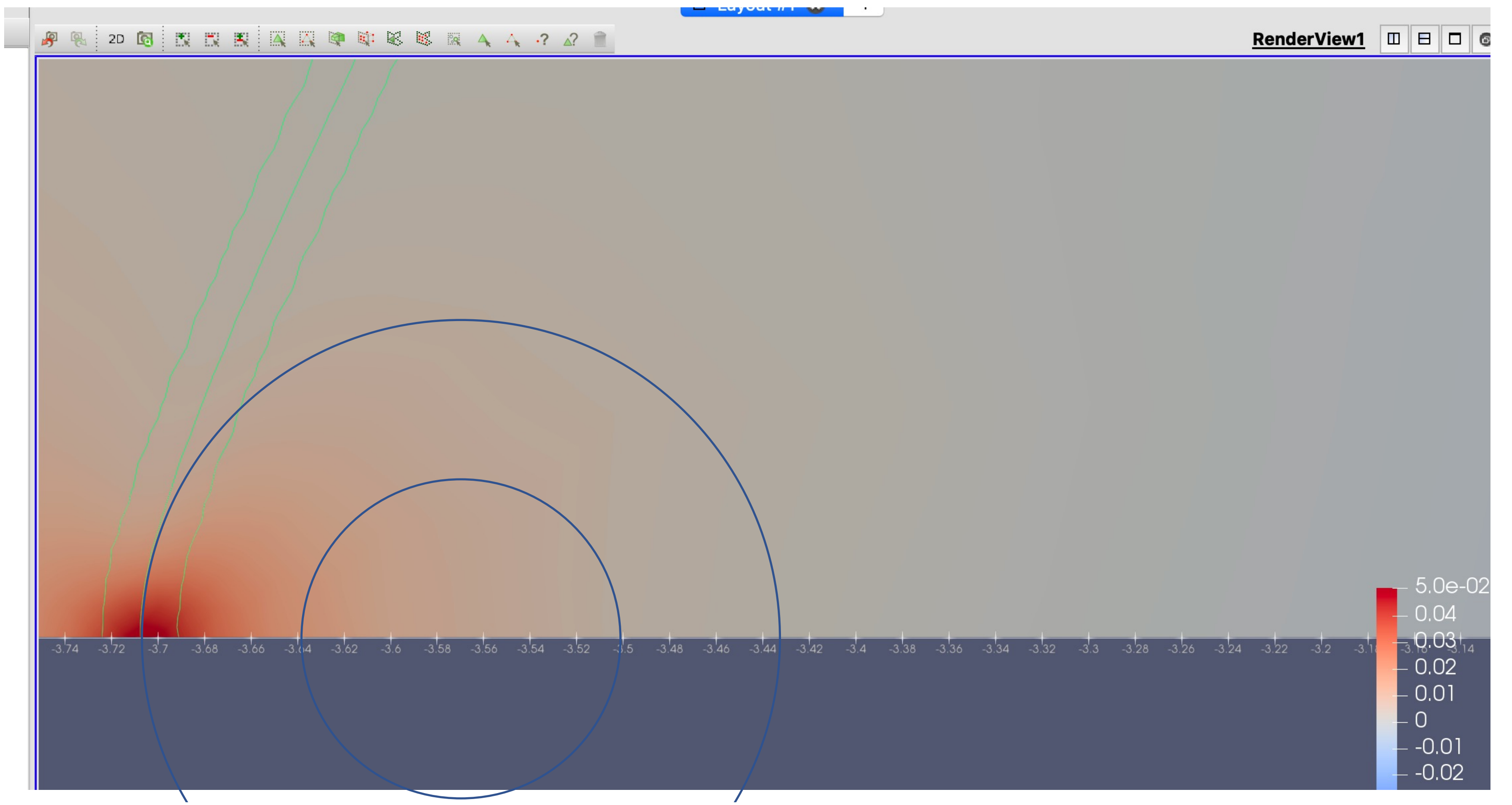
/Users/gustava2/prog/paradapt-2.4/Couette_wetting/P100_cn01

Wall speed = +- 0.05

Ca= 1.06*0.02=0.053



```
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P100_cn01/out           < outplotfile
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1E-11        < CG-tolerance
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0.0          < eps_c
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0.01          < xi
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0.99          < a
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0.3                                    < dr
0.05         <ui    use as wall speed
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```
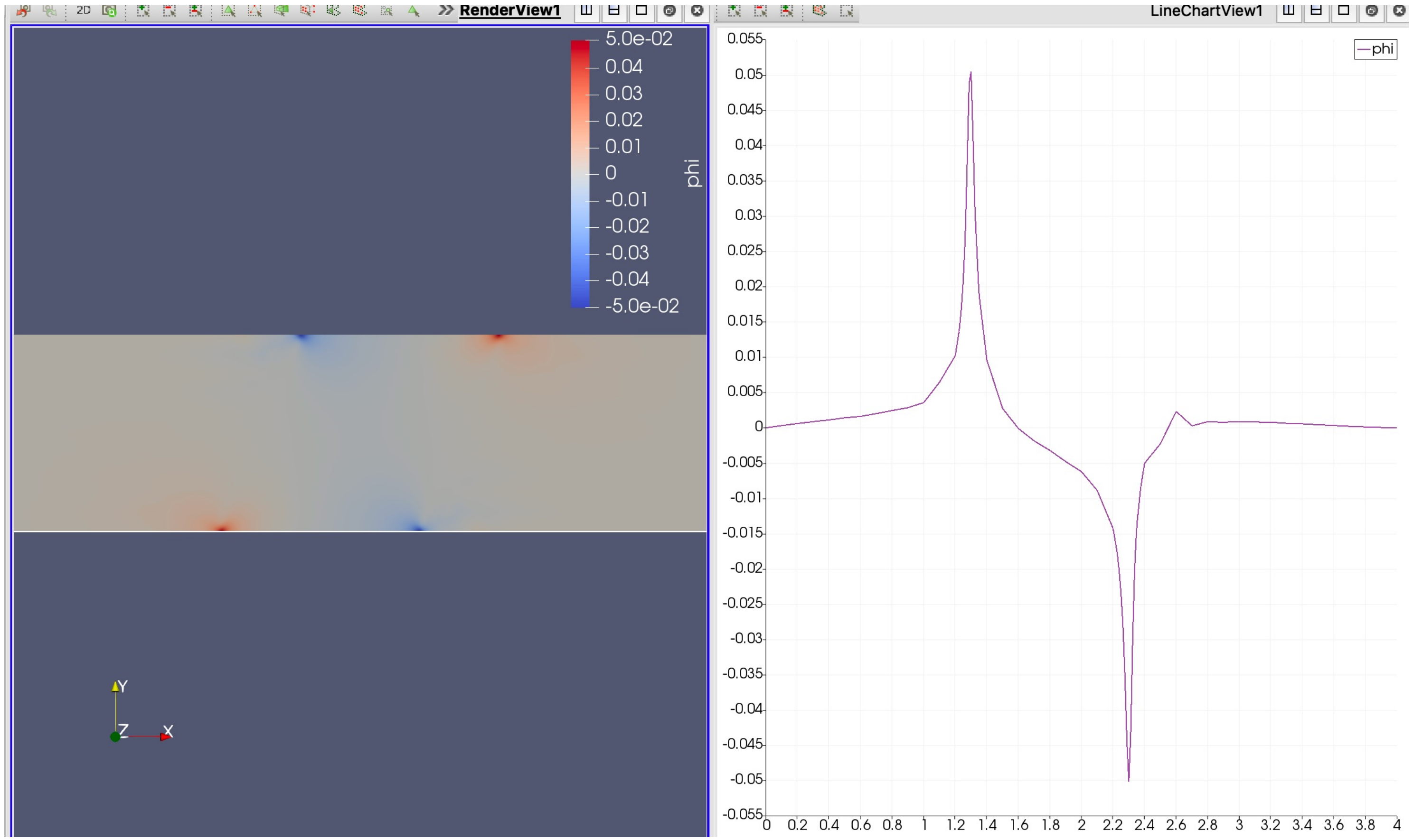

/Users/gustava2/prog/paradapt-2.4/Couette_wetting/P100_cn01

Wall speed = +- 0.05

Ca= 1.06*0.02=0.053



Cn	Pe
0.04	30
0.02	30
0.01	30
0.005	30
0.04	100
0.02	100
0.01	100
0.005	100
0.04	300
0.02	300
0.01	300
0.005	300
0.005	50
0.01	100
0.02	200
0.04	400
0.1	160
0.04	160
0.02	160
0.01	160
0.005	160

Made a number of simulations for Ca=0.053

Evaluated max chem pot value phi, and local curvature at the contact line

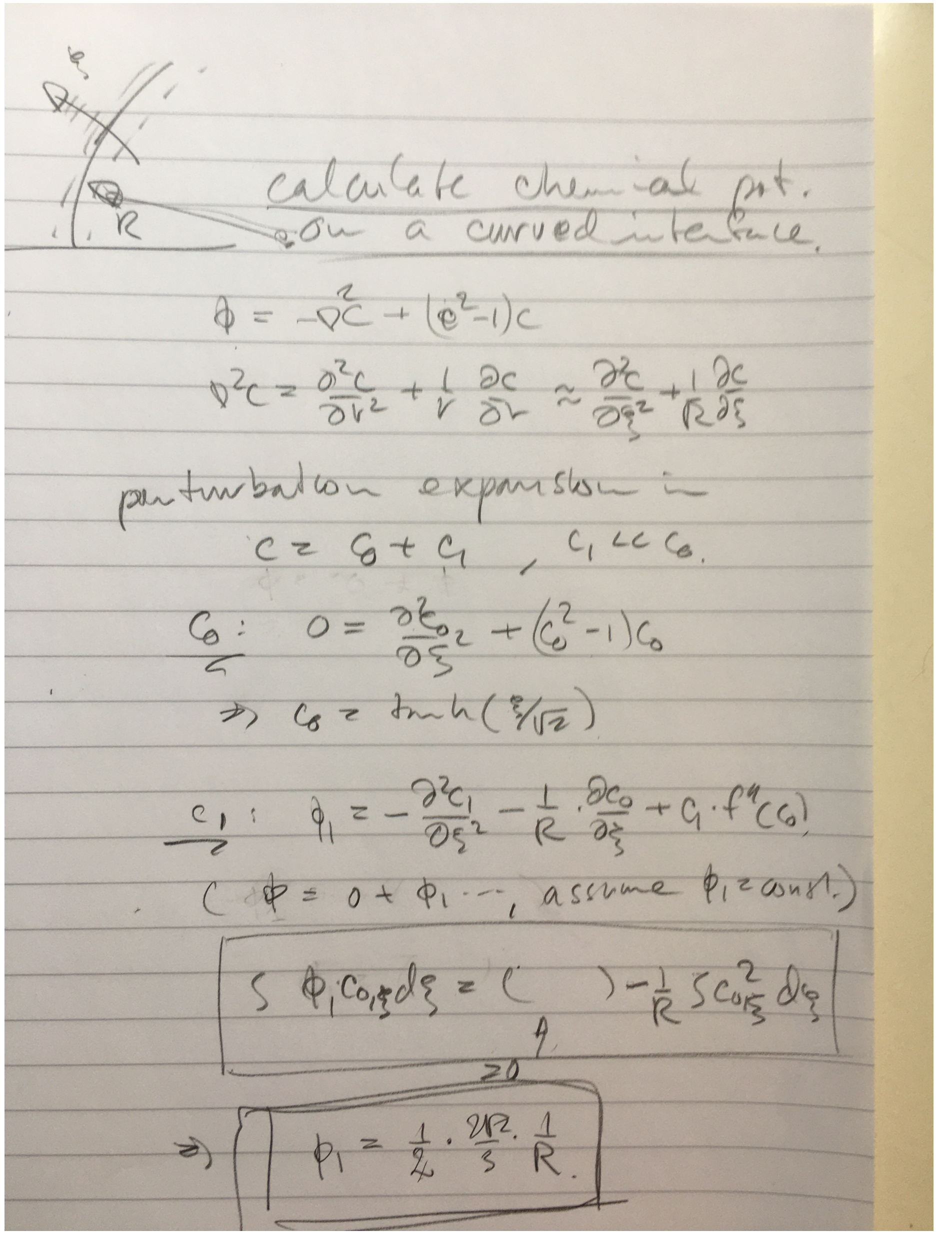
Mass diffusion moves the contact line right at the wall.

Try to relate the chemical potential to interface curvature and massflux of one species

Curved interface at equilibrium:

Result for radius of curvature *R*

$$\phi = \frac{1}{2}\frac{2\sqrt{2}}{3}\;\frac{Cn}{R}$$

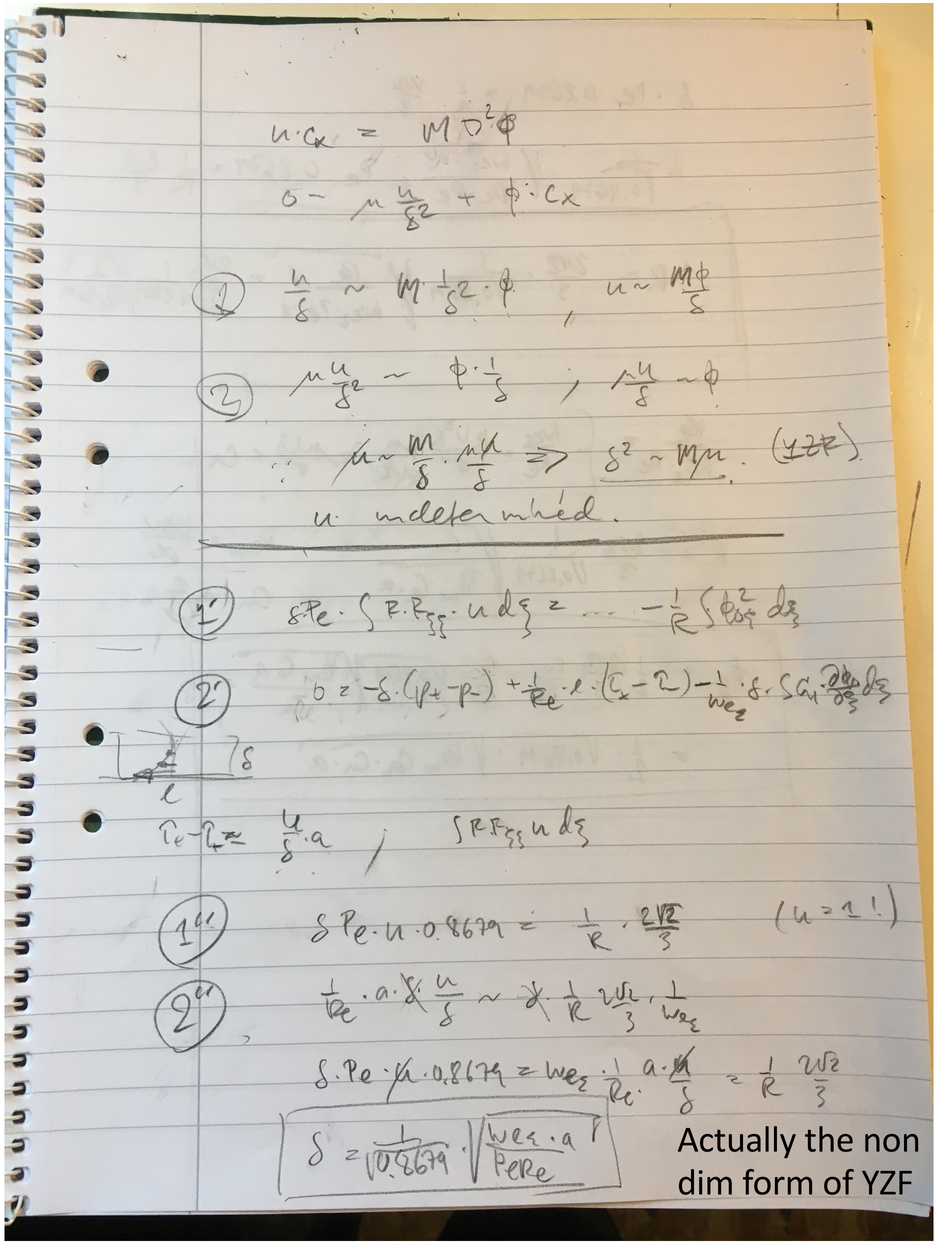


Mass diffusion moves the contact line right at the wall.

Try to relate the chemical potential to interface curvature and massflux of one species

Massflux?
A more daring attempt!

Mimick the scaling of YZF.



Mass diffusion moves the contact line right at the wall.

Try to relate the chemical potential to interface curvature and massflux of one species

Massflux?
A more daring attempt!

$$-U \cdot c_\xi \cdot Pe = \frac{\partial^2}{\partial \xi^2}\left(-\frac{\partial^2 c}{\partial \xi^2} + f'(c) - \frac{1}{R}\frac{\partial c}{\partial \xi}\right)$$

$$c = c_0 + c_1 \quad , \quad c_1 \ll 1$$

$$Pe = \frac{U\varepsilon}{\alpha} = \{\varepsilon = \text{i-f width}\} \ll 1$$

$$\underline{c_0 = \tanh(\xi/\sqrt{2})}$$

c_1? Find a similar Fredholm alternative?

introduce $R = \int^{\xi} \phi_0 \, d\xi$:

$$\frac{\partial R}{\partial \xi} = \phi_0 .$$

$$\Rightarrow \delta \int R(+U \cdot Pe \cdot R_{\xi\xi}) d\xi = \int \phi_{1\xi} \cdot (\underbrace{\phi_{\xi\xi} - \ldots}_{=0}) d\xi - \int \frac{1}{R} \cdot R \cdot R_{\xi\xi\xi\xi} \, d\xi$$

$$\Rightarrow \boxed{\delta \, U_{cl} \cdot Pe \cdot 2\sqrt{2}(1 - \ln 2) = \frac{2\sqrt{2}}{3} \cdot \frac{1}{R}.}$$

or $$\boxed{-U_{cl} \delta Pe \cdot 0{,}8679 = \frac{1}{R} \cdot 0{,}9428}$$

or $$-U_{CL} \delta Pe_w \cdot 0.8679 = \frac{1}{R_w} \cdot 0.9428$$

$$Pe_w = \frac{UW}{\alpha} \; , \; R_w = \frac{R^*}{W}.$$

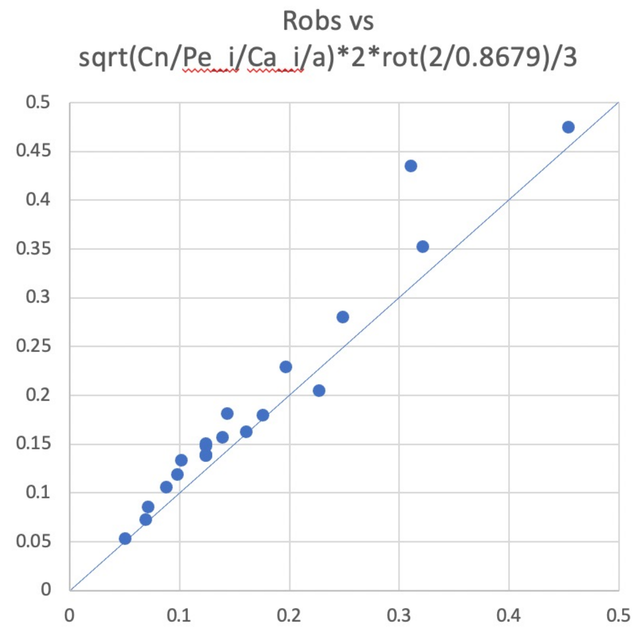
Mass diffusion moves the contact line right at the wall.

Try to relate the chemical potential to interface curvature and massflux of one species

End result:

Local curvature at CL as a function of parameters

$$R = \frac{2\sqrt{2}}{3}\,\frac{1}{\sqrt{0.8679}}\sqrt{\frac{Cn}{Pe\;Ca\;a}}$$



Geometry factor for the viscous flow
a = 2.5
Could/should depend on the static contact angle

Mass diffusion moves the contact line right at the wall.

Try to relate the chemical potential to interface curvature and massflux of one species

End result:

Local curvature at CL as a function of parameters

$$R = \frac{2\sqrt{2}}{3} \; \frac{1}{\sqrt{0.8679}} \sqrt{\frac{Cn}{Pe\ Ca\ a}}$$

$$Cn = \frac{\varepsilon}{W}$$

$$Pe = \frac{UW}{\alpha}$$

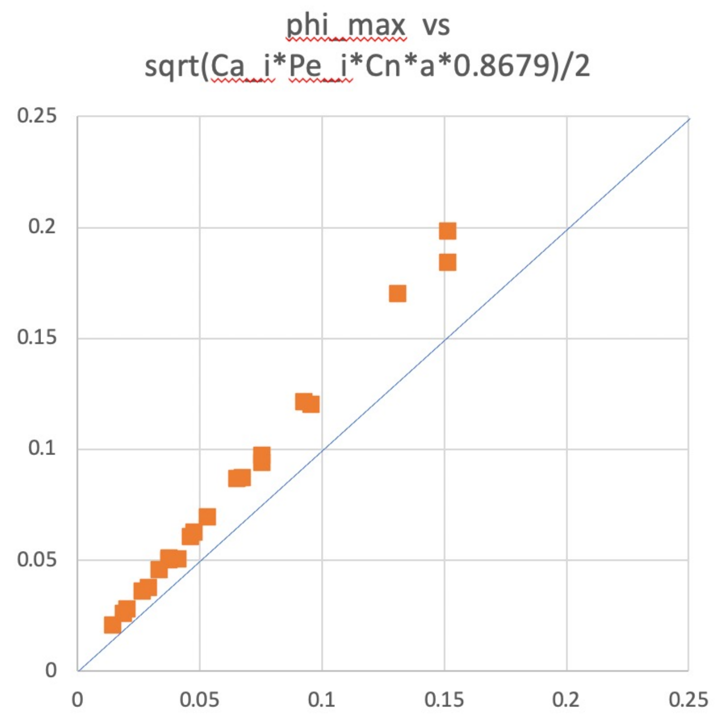
$$Ca = \frac{\mu U}{\gamma}$$

Mass diffusion moves the contact line right at the wall.

Try to relate the chemical potential to interface curvature and massflux of one species

Chemical potential:

$$\phi = \frac{\sqrt{0.8679}}{2} \sqrt{Pe_W \, Ca \, Cn \, a}$$

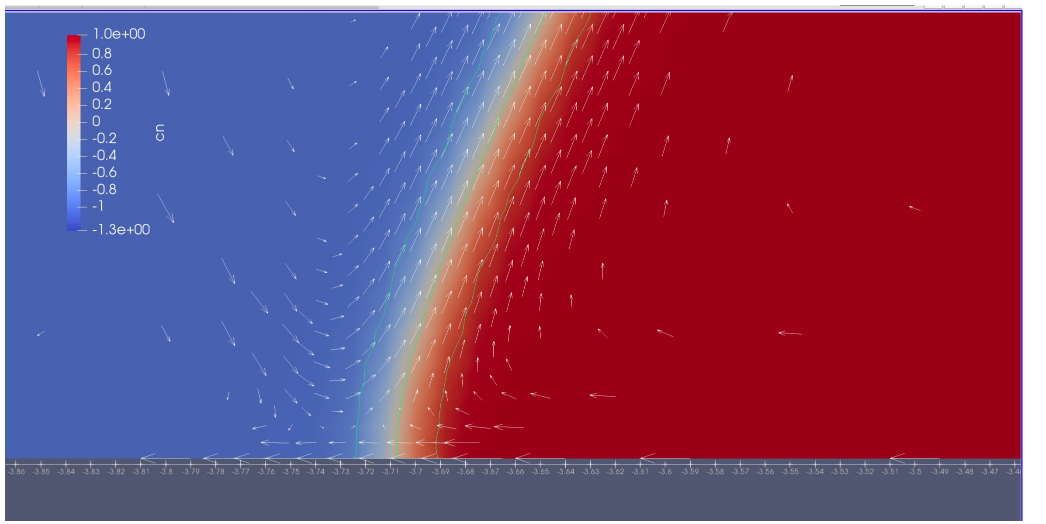


Toy model that mimicks PF (at lower cost?)

Sharp-interface limit of the Cahn-Hilliard
model for moving contact lines
Yue, Zhou, Feng JFM 2010

Scaling gives

Stagnation point at $\sqrt{\kappa\mu}$
PF mobility and viscosity.
Independent of interface width.
$\sqrt{\kappa\mu}$ works as a slip length



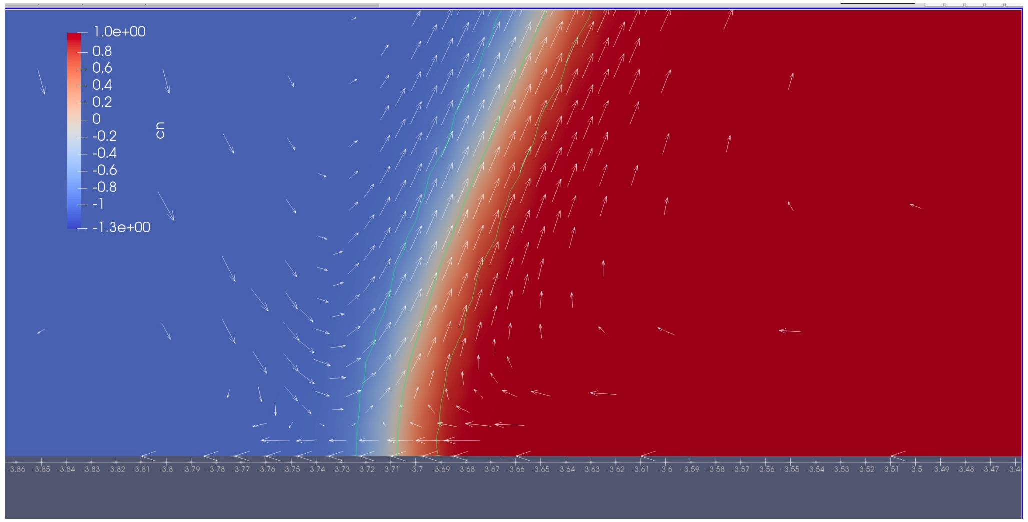
Toy model that mimicks PF (at lower cost?)

Use as slip length

$$\delta = \frac{1}{\sqrt{0.8679}}\sqrt{\frac{Ca\ Cn\ a}{Pe}}$$

And an apparent contact angle

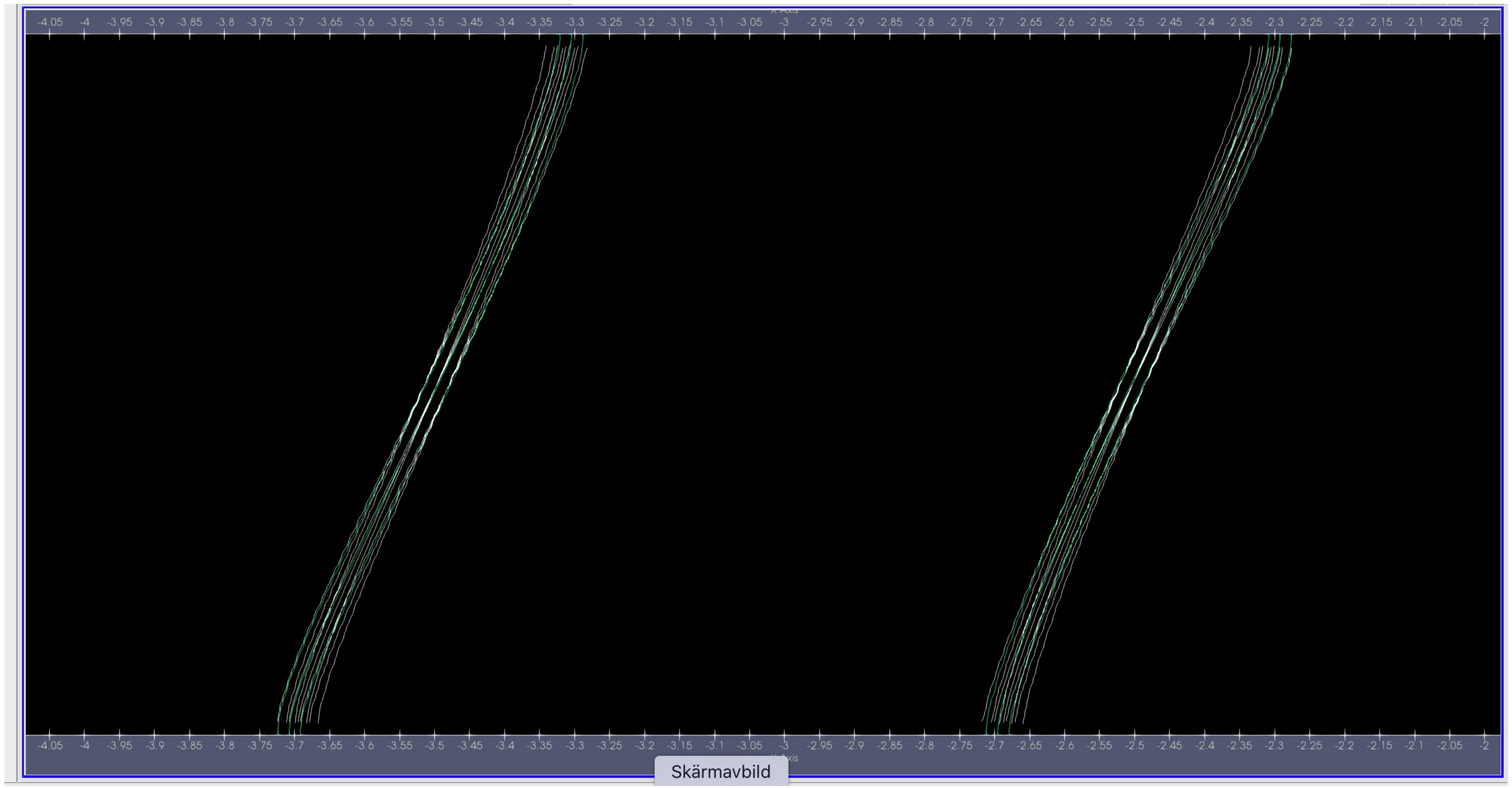
$$cos\theta_a = cos\theta_s + \frac{3}{2\sqrt{2}}\ Ca\ a$$



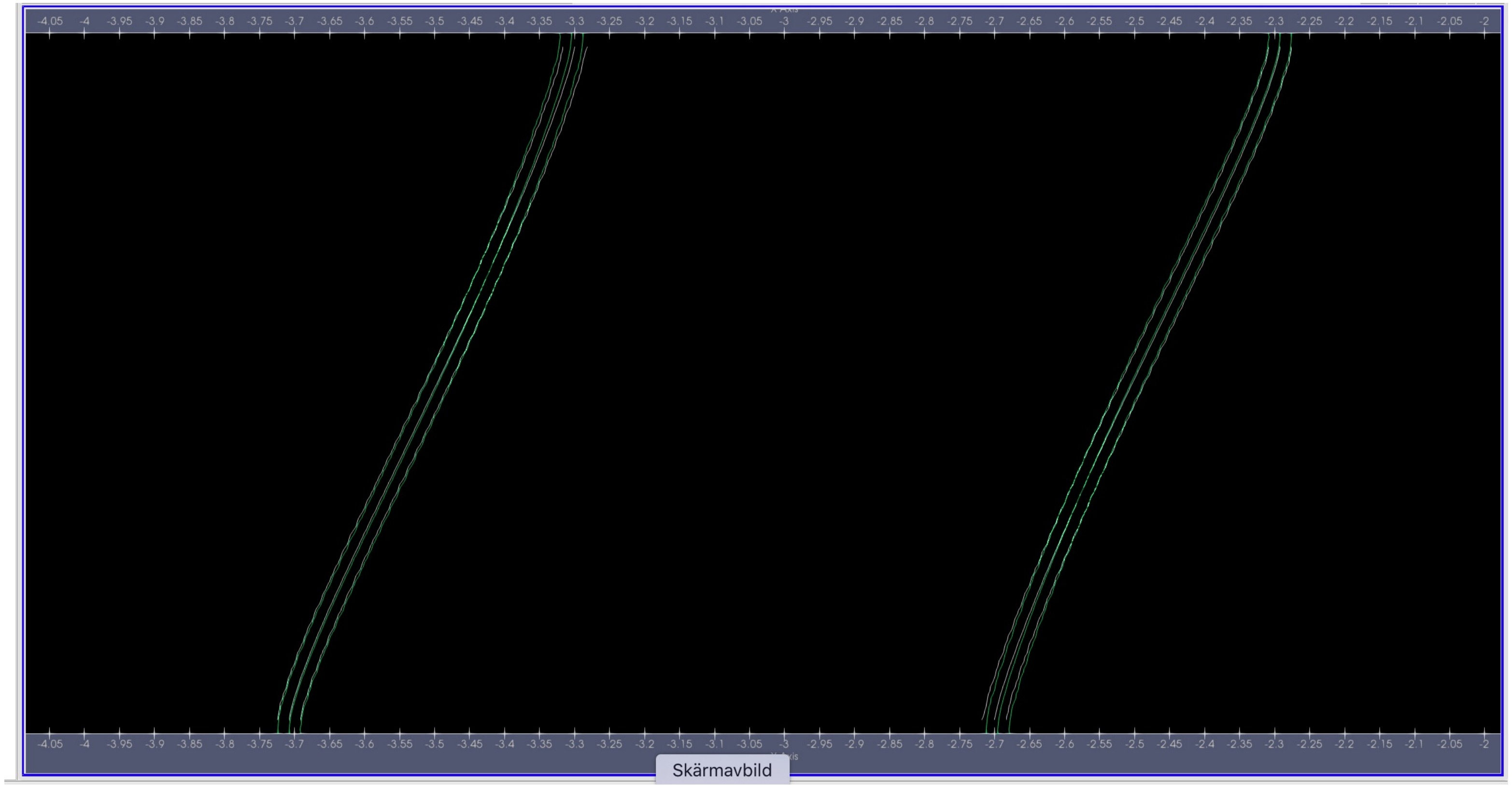
(Obtained from local curvature

$$R = \frac{2\sqrt{2}}{3}\ \frac{1}{\sqrt{0.8679}}\sqrt{\frac{Cn}{Pe\ Ca\ a}})$$

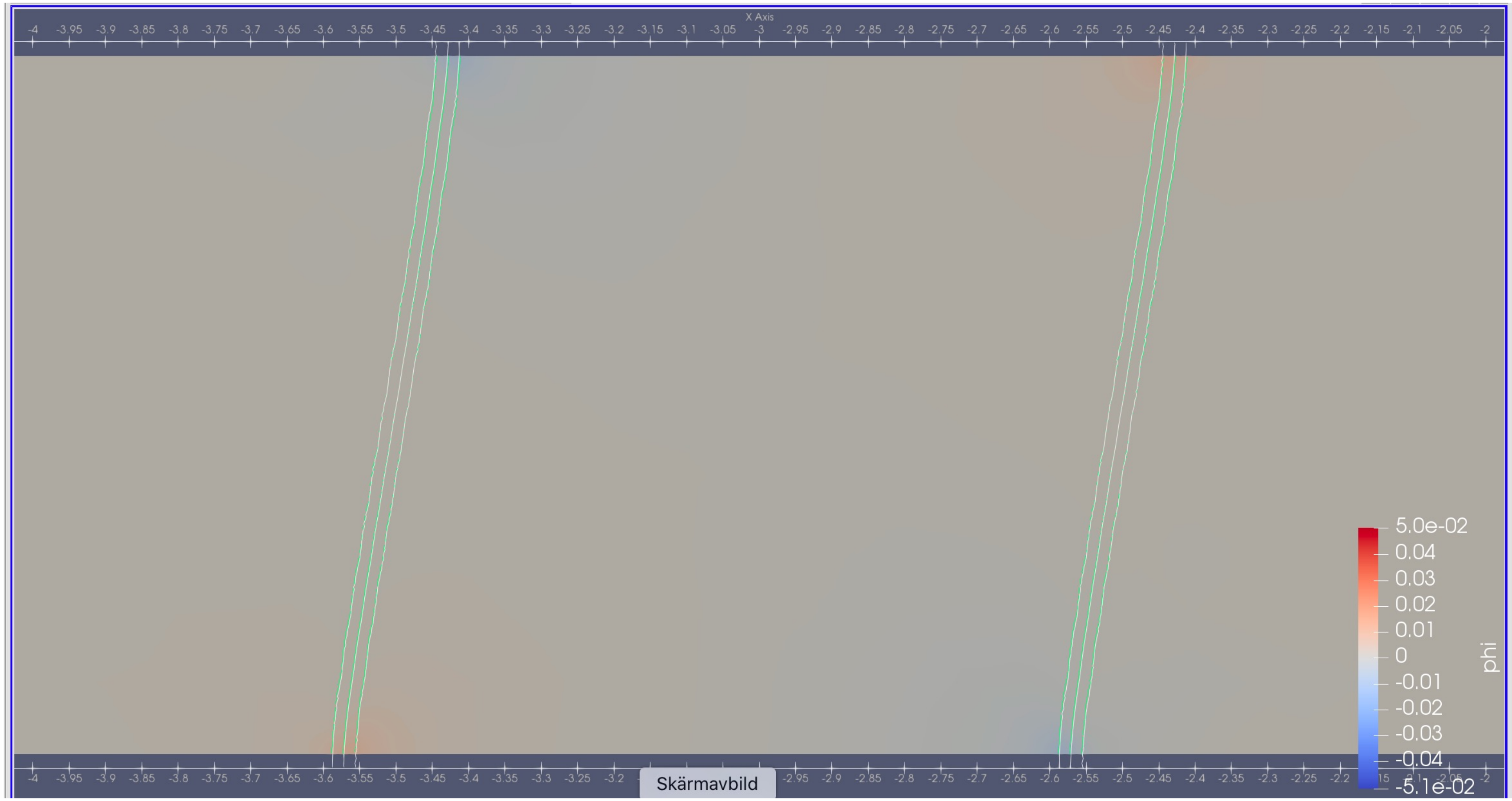
P100_cn01	full PF
toyP100_01_a2	a=2.0
toyP100_01	a=2.5
toyP100_01_a3	a=3.0



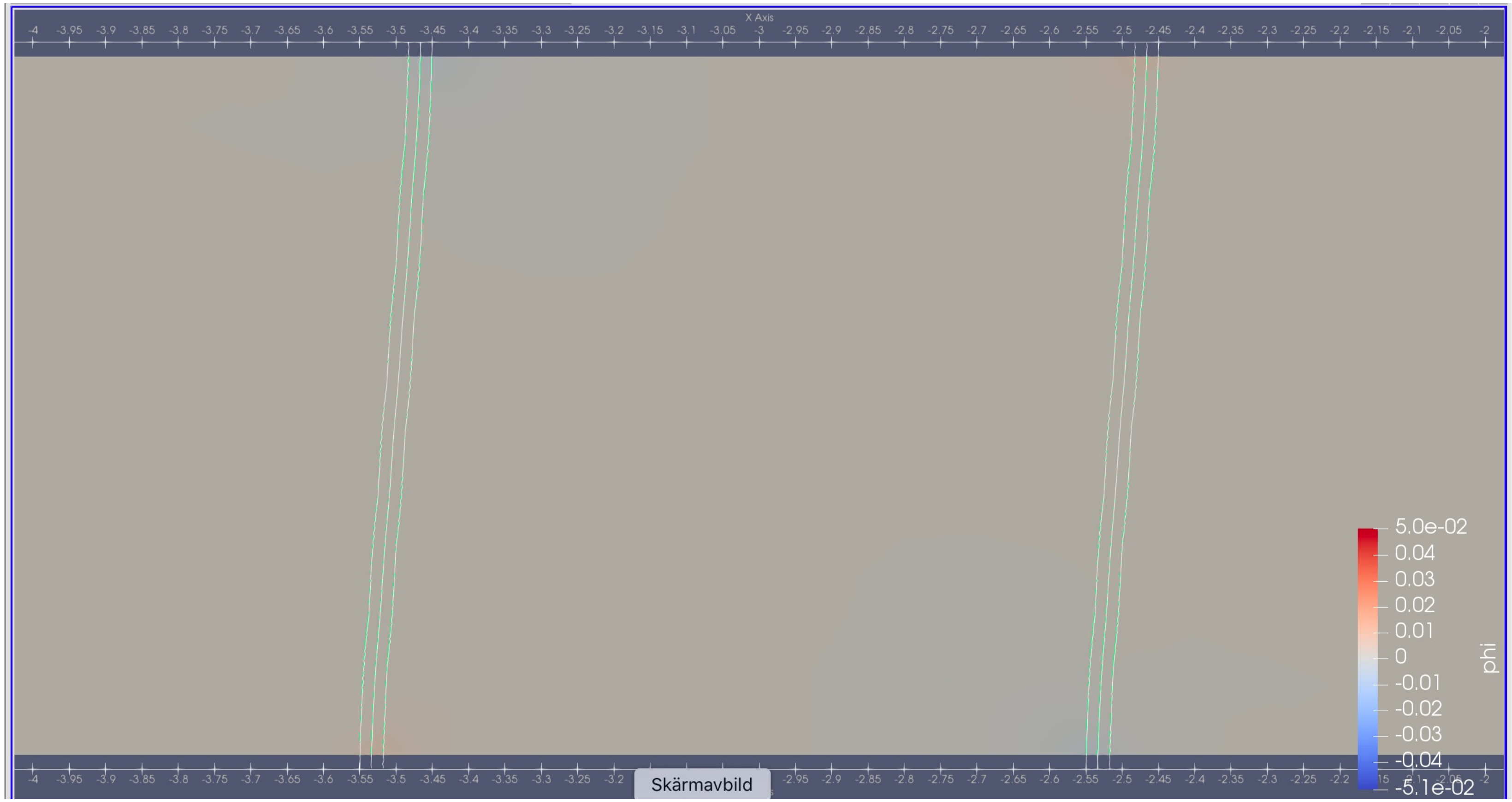
P100_cn01	full PF
toyP100_01_a2	a=2.0
toyP100_01	a=2.5
toyP100_01_a3	a=3.0 best fit



P1c1_Ca02
t1c1_Ca02

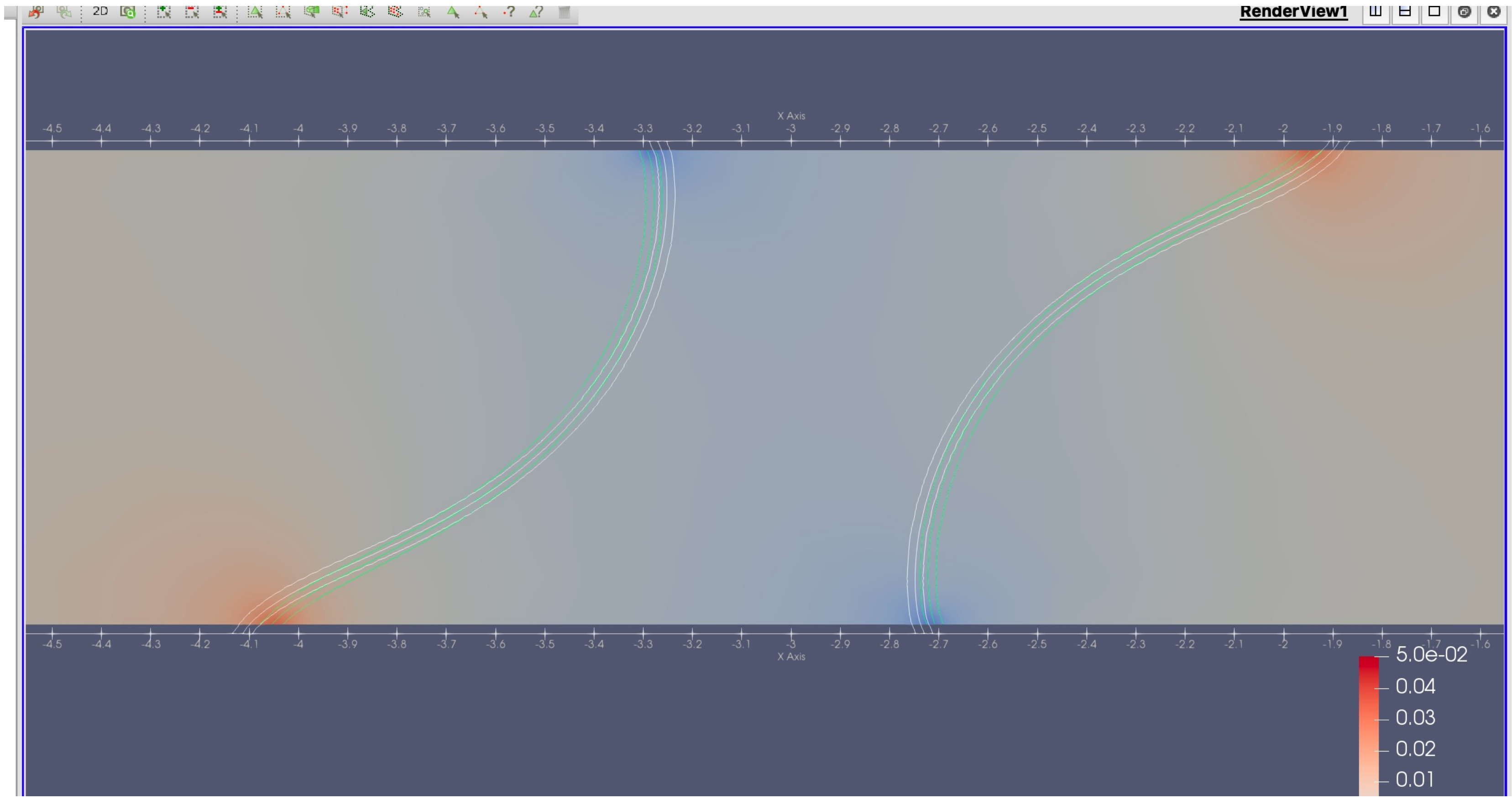


P1c1_Ca01
t1c1_Ca01



P1c1_Ca05_th60
t1c1_Ca05_th60 a=3

Ca =0.053
theta_s = 60 deg



P1c1_Ca02_th60
t1c1_Ca02_th60 a=3

Ca =0.0212
theta_s = 60 deg