Rheology of active and inactive liquid crystals

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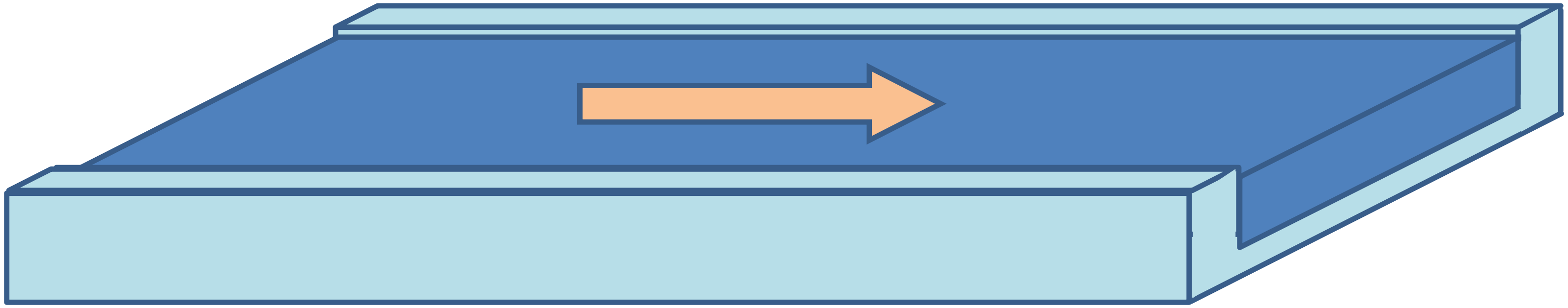
Rheology of liquid crystals

- Mathematical model of active/inactive nematics in a shallow channel
- What are the steady distortion/flow modes?
- Which modes are stable?
- How are these modes affected by an applied pressure gradient?
- How are these modes affected by surface preferred orientations?
- Can we design pressure gradient/surface orientations to select modes?



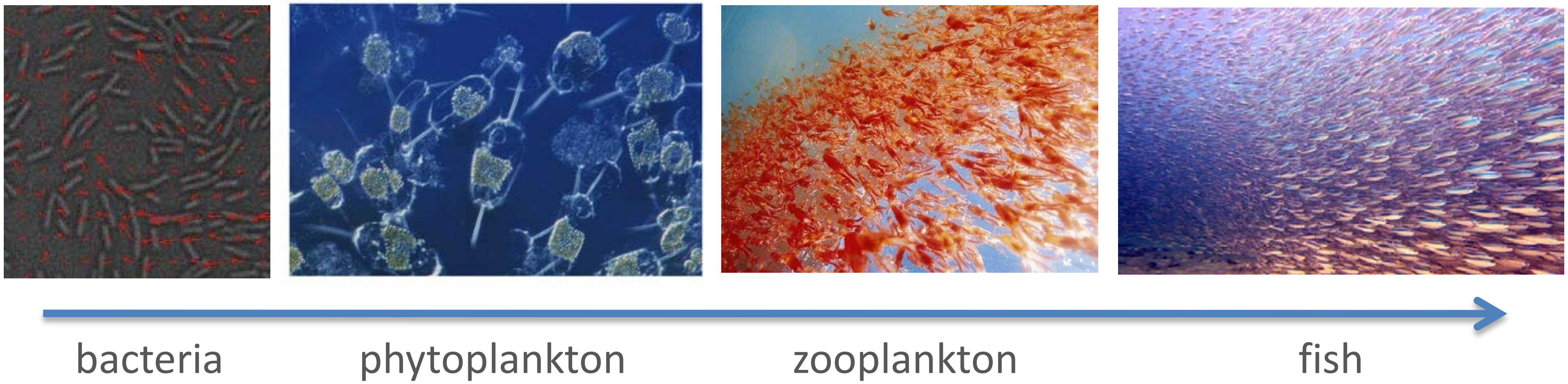
From inactive to active liquid crystals

Isotropic liquids flow through external influences (i.e. shear, pressure, gravity)

“Inactive” liquid crystals (standard molecular liquid crystals) can induce flow, but only when out of equlibrium (i.e. backflow).

Active liquid crystals consist of objects (i.e. living organisms not molecules) which form a nematic phase and also have the ability to produce energy internally.

This normally means they can “**swim**” and induce flow in the surrounding fluid.



Activity produces complex behaviour

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Control of active liquid crystals with a magnetic field

Pau Guillamat[a,b], Jordi Ignés-Mullol[a,b], and Francesc Sagués[a,b,1]

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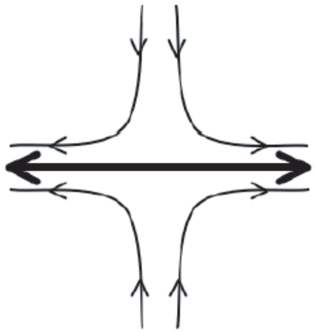
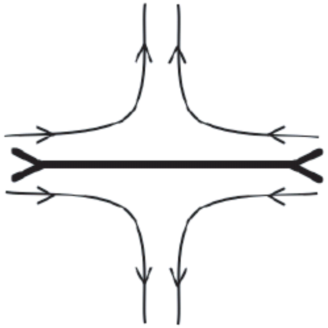
Active nematics

- **Continuum hydrodynamic models** based on liquid crystal theory have been used to describe active nematics.
- These systems swim in patterns that suggest **long-range collective ordering**.
- The activity in these systems relies on **continuous energy production** (and expenditure) by the individual particles.
- They then **generate forces on each other** and/or the surrounding fluid.



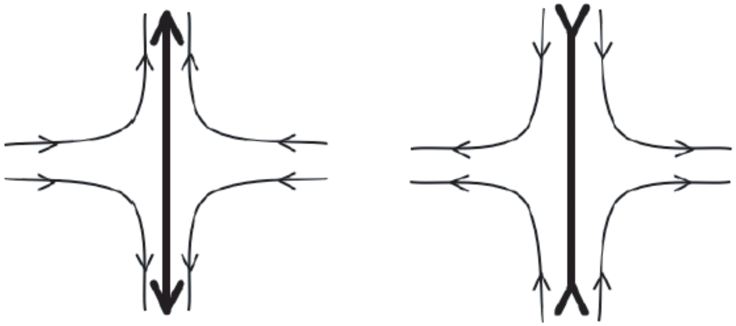
extensile (pushers)



contractile (pullers)

Active nematics

- We think of the “swimming” organisms as either “pushers” or “pullers”



$\zeta < 0$

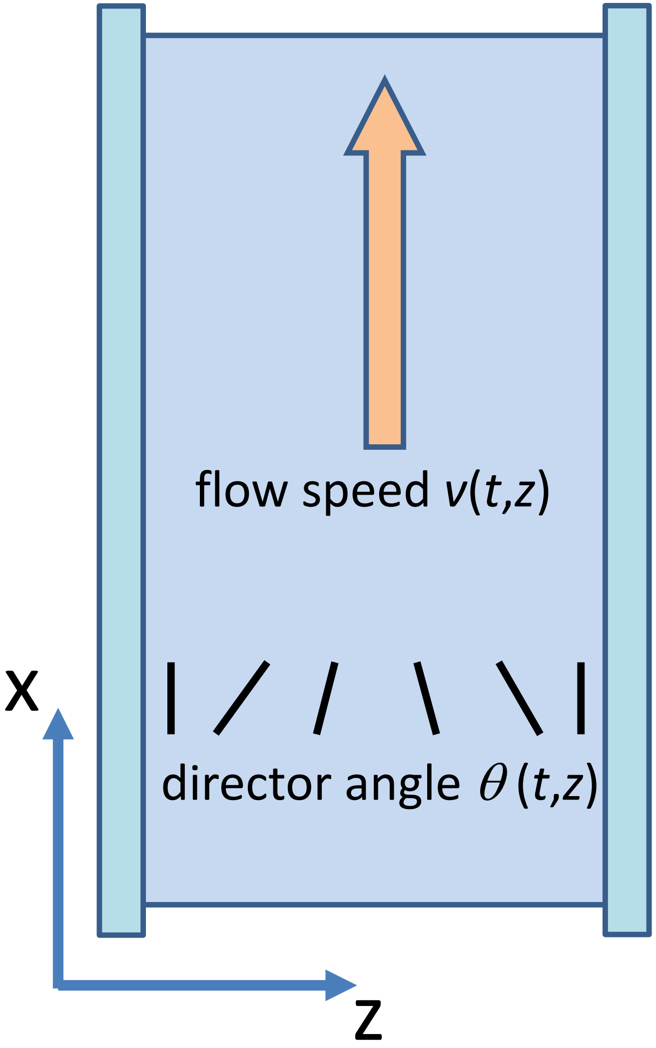
extensile (pushers)

$\zeta > 0$

contractile (pullers)

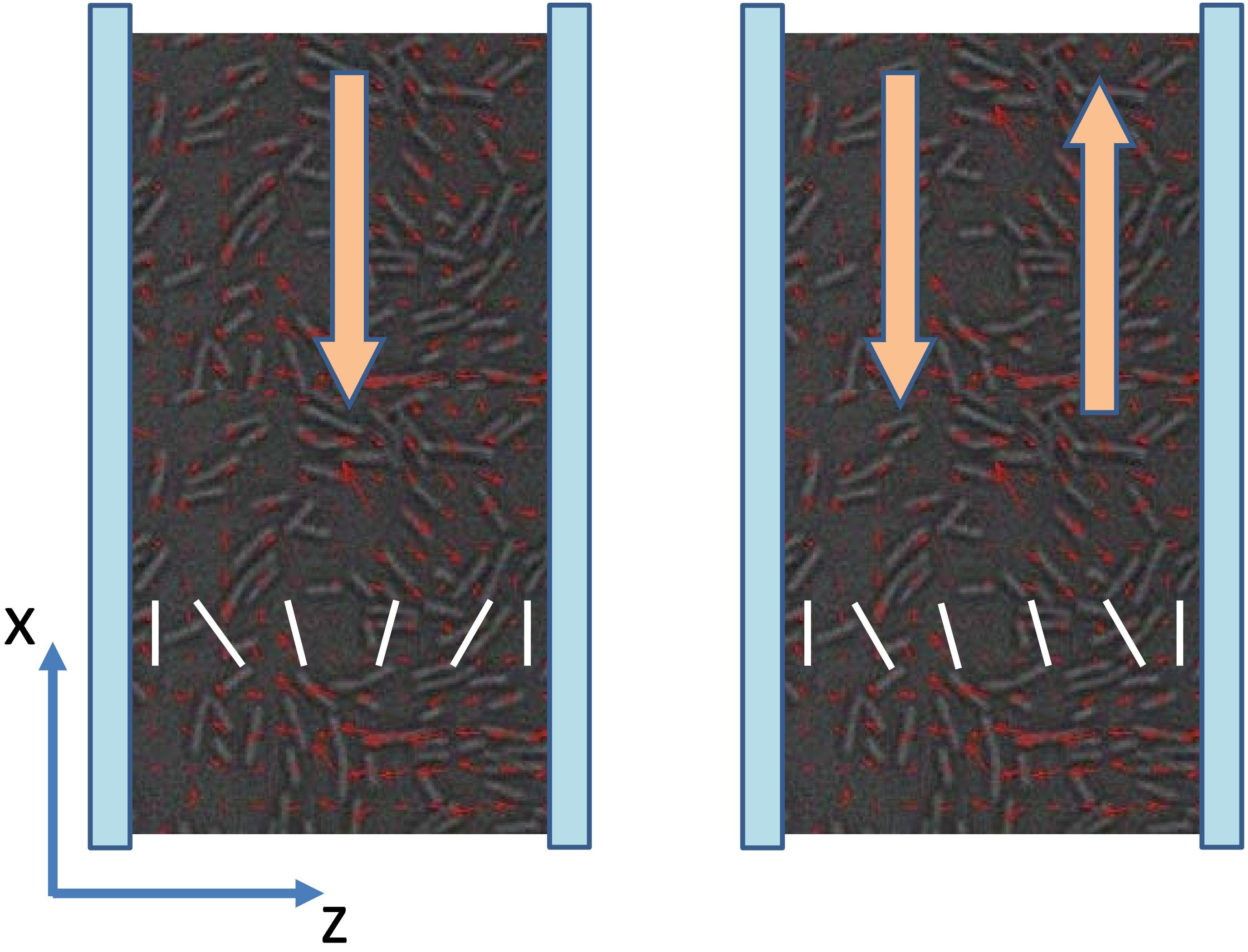
- The simplest model uses the Ericksen-Leslie theory with just one extra term in the stress tensor
- The stress tensor is written as $\tau = \tau_{nem} + \underbrace{\boxed{\zeta\left(\mathbf{n}\otimes\mathbf{n}\right)}}_{\text{activity}}$
- We consider flow aligning organisms (similar states occur in tumbling regimes).

System geometry



- flow in the x-direction only
- director in plane of shallow channel
- speed and director angle depend on the cross-channel coordinate, z
- fixed director orientation at the channel sides
- we may impose a pressure gradient in the x-direction and director tilt at the sides

System geometry



Active nematics

Governing equations are,

angular momentum

$$\gamma_1\theta_t = (K_1\cos^2\theta + K_3\sin^2\theta)\theta_{zz} + (K_3 - K_1)\sin\theta\cos\theta(\theta_z)^2 - m(\theta)v_z,$$

$$\rho v_t = (g(\theta)v_z + m(\theta)\theta_t + \zeta\cos\theta\sin\theta)_z$$

linear momentum

where,

$$m(\theta) = \alpha_3\cos^2\theta - \alpha_2\sin^2\theta,$$

rotation and stretching viscosity

$$g(\theta) = \frac{1}{2}\left(\alpha_4 + (\alpha_5 - \alpha_2)\sin^2\theta + (\alpha_3 + \alpha_6)\cos^2\theta\right) + \alpha_1\sin^2\theta\cos^2\theta.$$

shear viscosity

Active nematics

director rotation

elastic terms

director-flow coupling

$$\boxed{\gamma_1 \theta_t} = \boxed{(K_1 \cos^2\theta + K_3 \sin^2\theta)\theta_{zz} + (K_3 - K_1)\sin\theta\cos\theta(\theta_z)^2} - \boxed{m(\theta)v_z,}$$

$$\boxed{\rho v_t} = \boxed{(g(\theta)v_z} + \boxed{m(\theta)\theta_t} + \boxed{(\zeta\cos\theta\sin\theta)_z}$$

flow inertia **fluid viscosity** **director-flow coupling** **activity**

where,

$$m(\theta) = \alpha_3 \cos^2\theta - \alpha_2 \sin^2\theta,$$

$$g(\theta) = \frac{1}{2}\left(\alpha_4 + (\alpha_5 - \alpha_2)\sin^2\theta + (\alpha_3 + \alpha_6)\cos^2\theta\right) + \alpha_1 \sin^2\theta\cos^2\theta.$$

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$$\boxed{\rho v_t} = \boxed{(g(\theta) v_z} + \boxed{m(\theta)\theta_t} + \boxed{\zeta \cos\theta \sin\theta)_z} - \boxed{\tilde{p}_x}$$

flow inertia

fluid viscosity

director-flow coupling

activity

applied pressure gradient

where,

$$m(\theta) = \alpha_3 \cos^2\theta - \alpha_2 \sin^2\theta,$$

$$g(\theta) = \frac{1}{2}\Big(\alpha_4 + (\alpha_5 - \alpha_2)\sin^2\theta + (\alpha_3 + \alpha_6)\cos^2\theta\Big) + \alpha_1 \sin^2\theta \cos^2\theta.$$

Active nematics

Decoupling of these two equations is possible...

$$\gamma_1\theta_t = (K_1\cos^2\theta + K_3\sin^2\theta)\theta_{zz} + (K_3 - K_1)\sin\theta\cos\theta(\theta_z)^2 - m(\theta)v_z,$$

$$\rho v_t = (g(\theta)v_z + m(\theta)\theta_t + \zeta\cos\theta\sin\theta)_z - \tilde{p}_x,$$

Active nematics

Decoupling of these two equations is possible...

$$\left(\gamma_1 - \frac{m^2(\theta)}{g(\theta)}\right)\theta_t = (K_1\cos^2\theta + K_3\sin^2\theta)\theta_{zz} + (K_3 - K_1)\sin\theta\cos\theta(\theta_z)^2 \\ - \frac{m(\theta)\mathcal{A}}{g(\theta)\mathcal{B}} + \frac{\zeta m(\theta)}{g(\theta)}\left[\cos\theta\sin\theta - \mathcal{K}_2 - \frac{\mathcal{C}}{\mathcal{B}}\right],$$

Active nematics

Decoupling of these two equations is possible...

director rotation (modified viscosity)

elastic terms

$$\boxed{\left(\gamma_1 - \frac{m^2(\theta)}{g(\theta)}\right)}\theta_t = \boxed{(K_1 \cos^2\theta + K_3 \sin^2\theta)\theta_{zz} + (K_3 - K_1)\sin\theta\cos\theta(\theta_z)^2}$$
$$- \boxed{\frac{m(\theta)\mathcal{A}}{g(\theta)\mathcal{B}}} + \boxed{\frac{\zeta m(\theta)}{g(\theta)}\left[\cos\theta\sin\theta - \mathcal{K}_2 - \frac{\mathcal{C}}{\mathcal{B}}\right]},$$

director-flow coupling

activity

where

$$\mathcal{A} = \int_0^d \frac{m(\theta)[(K_1\cos^2\theta + K_3\sin^2\theta)\theta_{zz} + (K_3 - K_1)\sin\theta\cos\theta(\theta_z)^2]}{\gamma_1 g(\theta) - m^2(\theta)}\,\mathrm{d}z,$$

$$\mathcal{B} = \int_0^d \frac{\gamma_1}{\gamma_1 g(\theta) - m^2(\theta)}\,\mathrm{d}z, \qquad \mathcal{K}_2 = \int_0^d \frac{\cos\theta\sin\theta}{g(\theta)}\,\mathrm{d}z \Big/ \int_0^d \frac{1}{g(\theta)}\,\mathrm{d}z.$$

$$\mathcal{C} = \int_0^d \frac{m^2(\theta)\cos\theta\sin\theta}{g(\theta)(\gamma_1 g(\theta) - m^2(\theta))}\,\mathrm{d}z - \mathcal{K}_2 \int_0^d \frac{m^2(\theta)}{g(\theta)(\gamma_1 g(\theta) - m^2(\theta))}\,\mathrm{d}z.$$

Active nematics

- The activity term is similar to a magnetic/electric field term…

$$\theta_t \sim \ldots \zeta\left(\cos\theta\sin\theta\int_{-1}^{1}\frac{1}{\hat{g}(\theta)} - \int_{-1}^{1}\frac{1}{\hat{g}(\theta)}\cos\theta\sin\theta\,dx\right)$$

…but a non-local version

- Positive and negative values of ζ will have different effects (help or hinder backflow/kickback, orient the director in different directions)

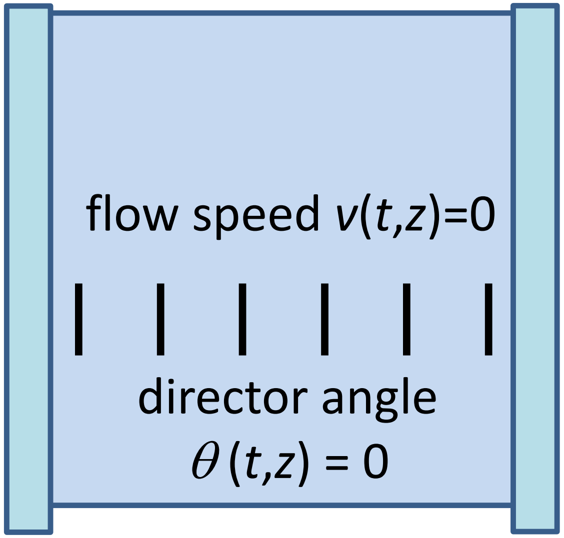
- This term has also introduced the possibility that the solution $\theta \equiv 0$ could be unstable.

Equilibrium solutions

Constant/trivial solution…

$$\left(\gamma_1 - \frac{m^2(\theta)}{g(\theta)}\right)\theta_t = (K_1\cos^2\theta + K_3\sin^2\theta)\theta_{zz} + (K_3 - K_1)\sin\theta\cos\theta(\theta_z)^2$$
$$-\frac{m(\theta)\mathcal{A}}{g(\theta)\mathcal{B}} + \frac{\zeta m(\theta)}{g(\theta)}\left[\cos\theta\sin\theta - \mathcal{K}_2 - \frac{\mathcal{C}}{\mathcal{B}}\right],$$

is a solution of this equation, (and leads to $v \equiv 0$)



flow speed $v(t,z)$=0

director angle

$\theta\,(t,z) = 0$

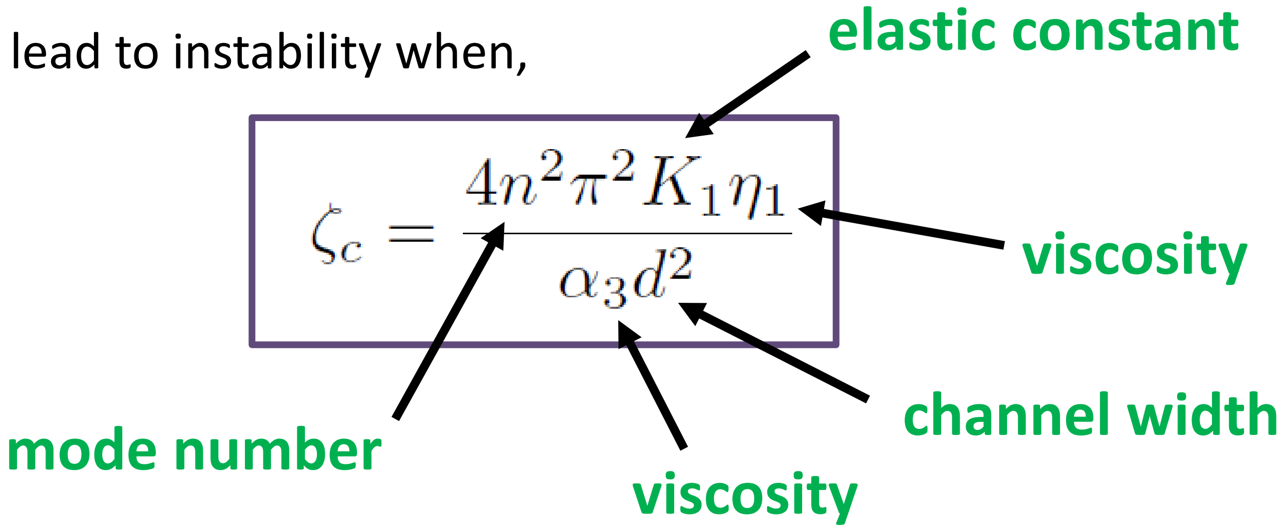
Equilibrium solutions

- Considering the stability of the state $\theta \equiv 0$ we see there are modes of instability

$$\text{Mode 1}: \theta(z,t) = \Theta\left[\cos\left(\frac{2q}{d}\left(z - \frac{d}{2}\right)\right) - \cos q\right]\exp(\sigma t),$$

$$\text{Mode 2}: \theta(z,t) = \Theta\sin\left(\frac{2n\pi z}{d}\right)\exp(\sigma t),$$

which **both** lead to instability when,



$$\boxed{\zeta_c = \frac{4n^2\pi^2K_1\eta_1}{\alpha_3 d^2}}$$

elastic constant

viscosity

channel width

mode number

viscosity

Equilibrium solutions

- Stability of $\theta \equiv 0$

$$\boxed{\zeta_c = \frac{4n^2\pi^2 K_1 \eta_1}{\alpha_3 d^2}}$$

- Equivalent to a Freedericksz transition (electric field induced)
- but **is “polarity” dependent**
- and the **critical parameter now involves viscosities**

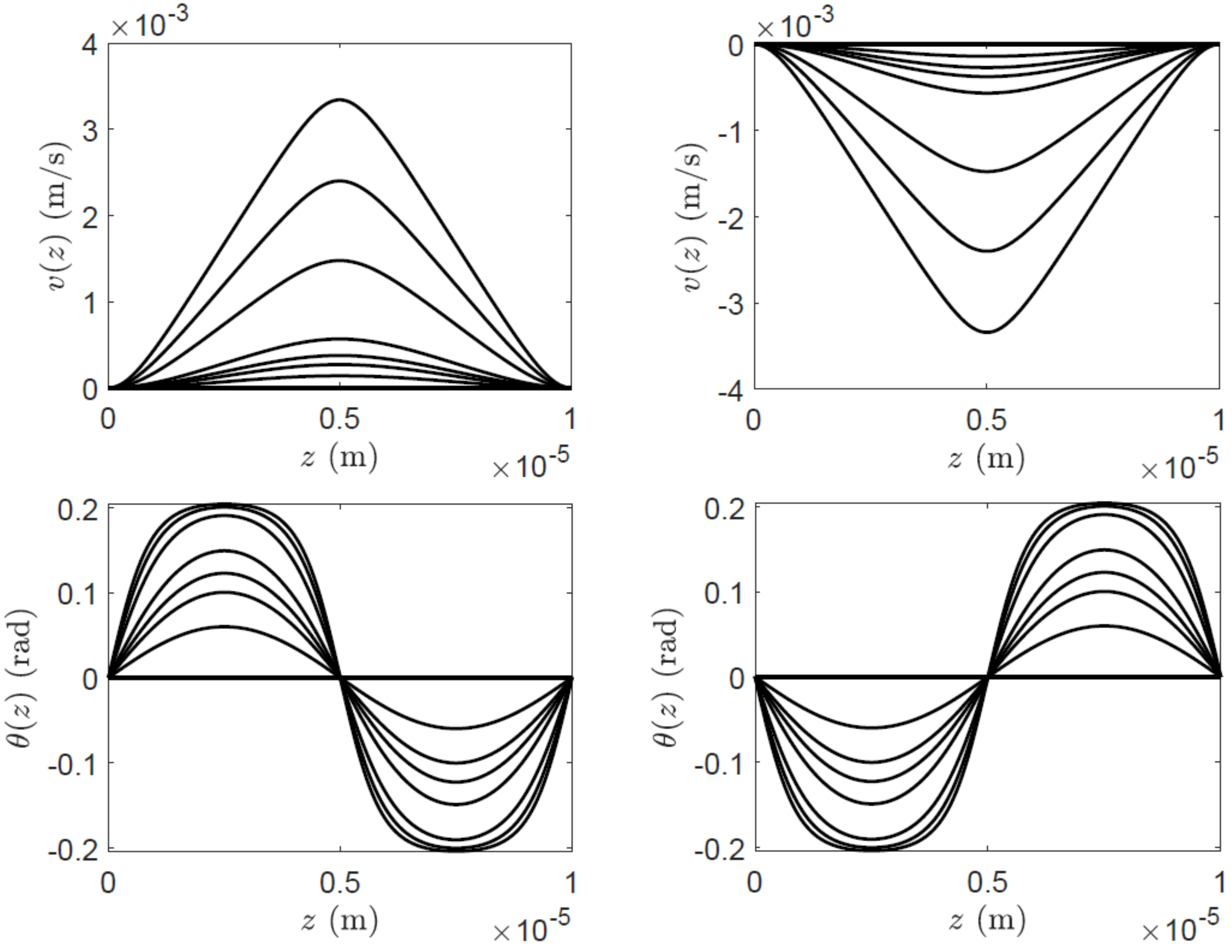
- and, particularly, depends on the sign of α_3
  - **rod-like pushers** will undergo a Freedericksz-like transition
  - **disc-like pullers** will undergo a Freedericksz-like transition

Equilibrium solutions

- What does the trivial state transition to?

symmetric flow

antisymmetric director



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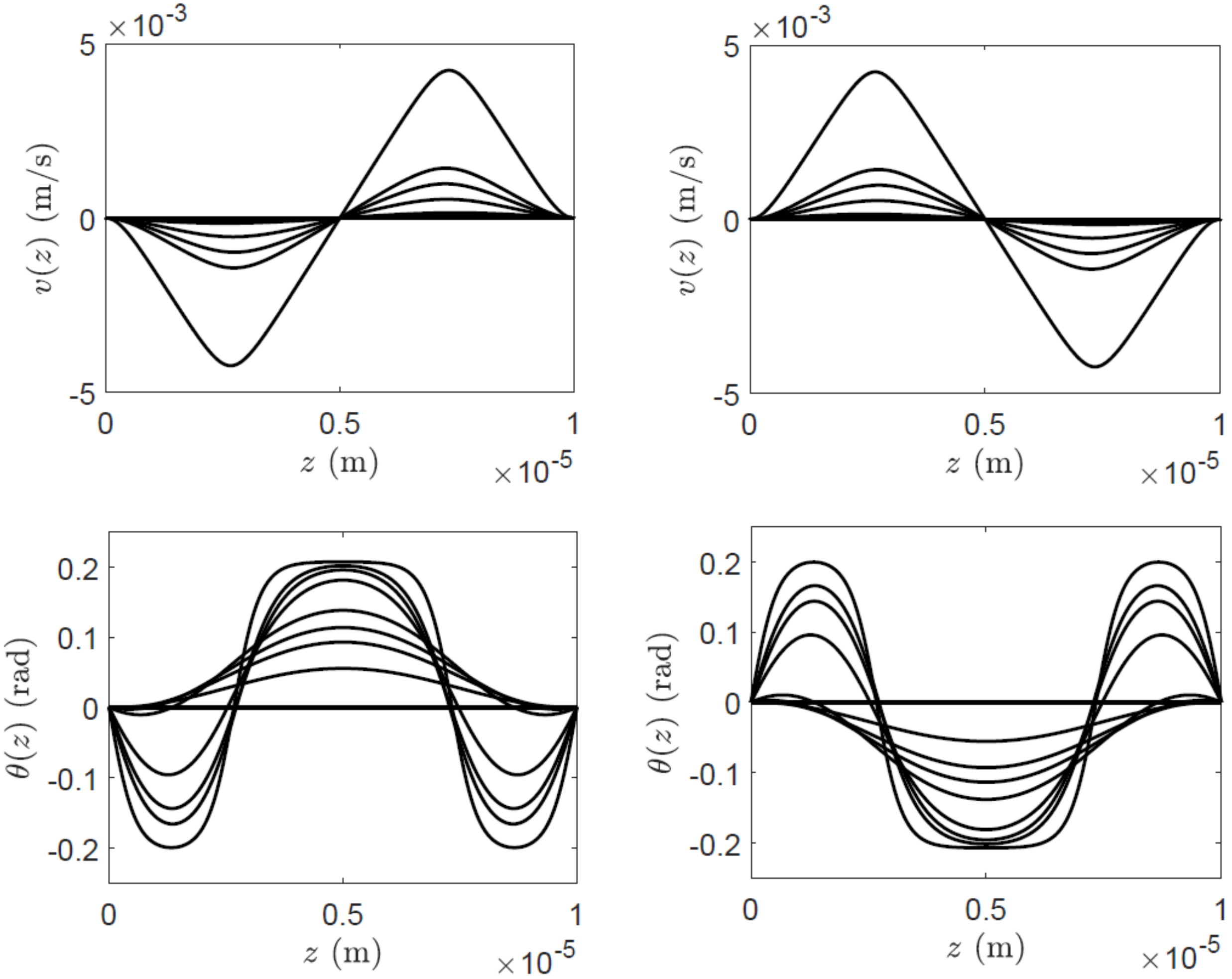
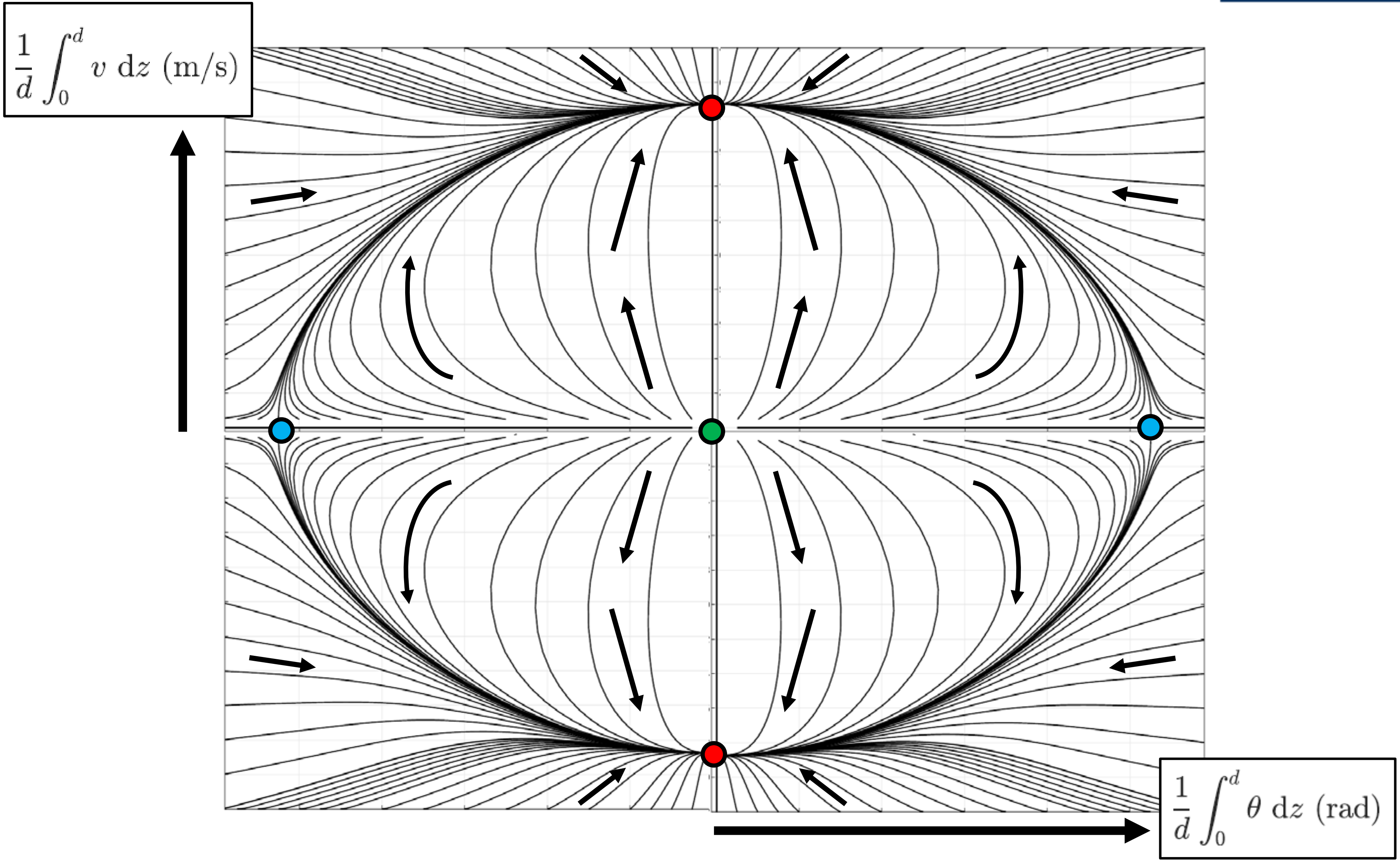


Equilibrium solutions

- We can map trajectories of the system in terms of two measures



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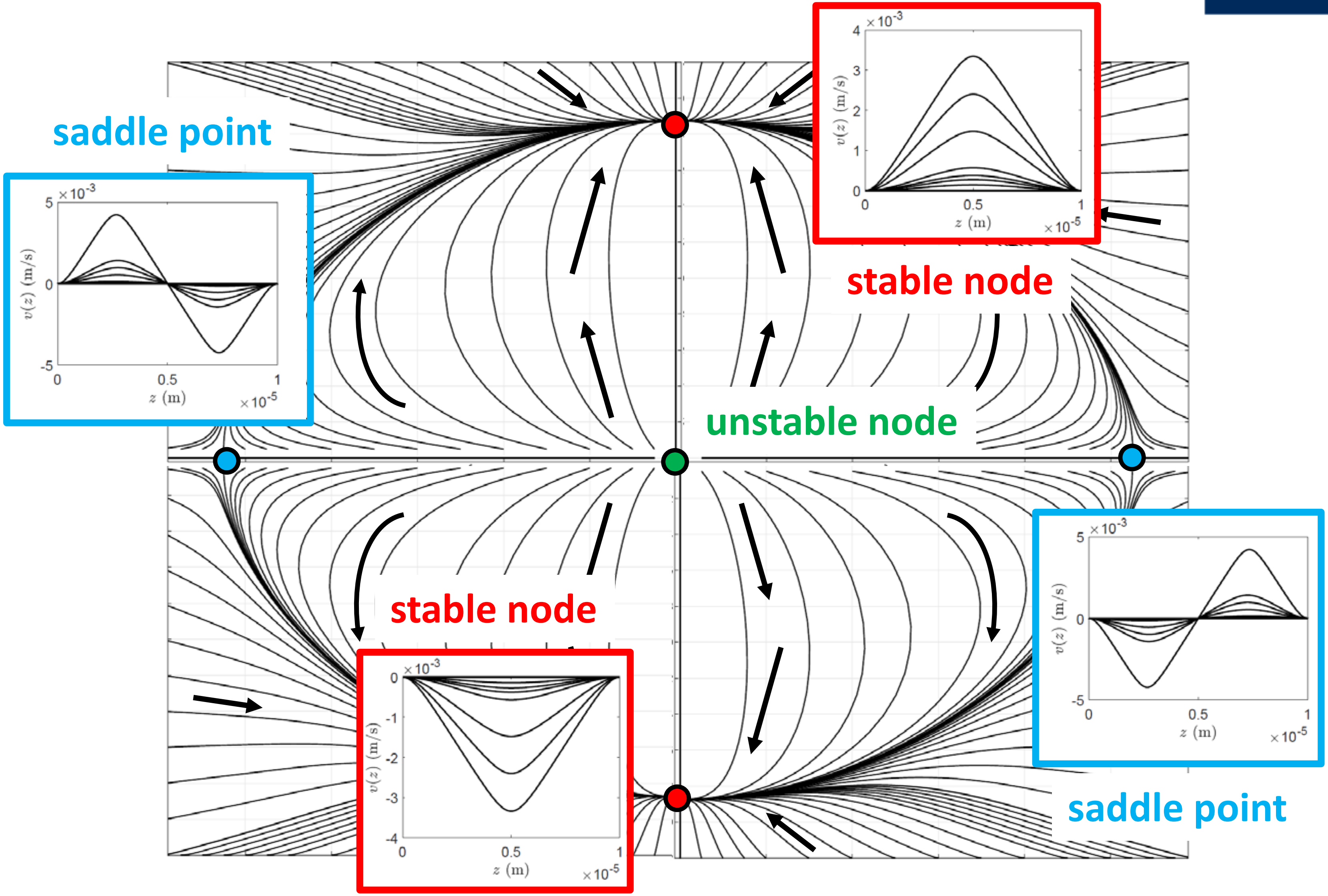

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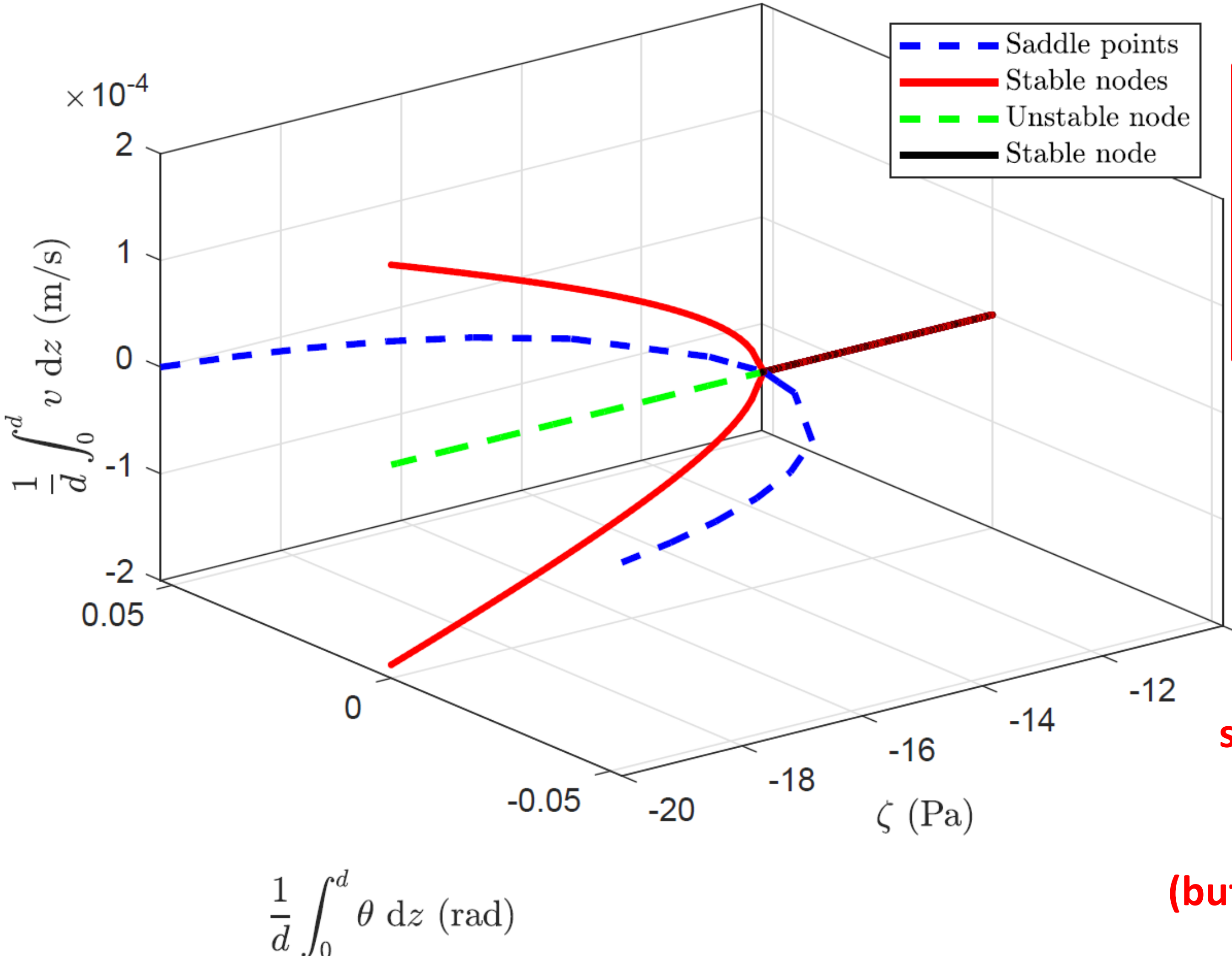
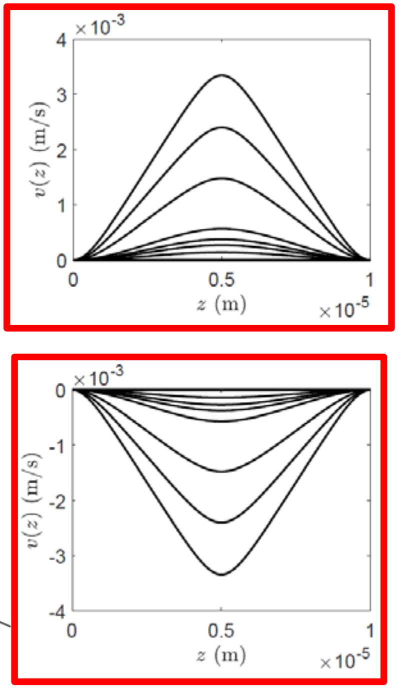


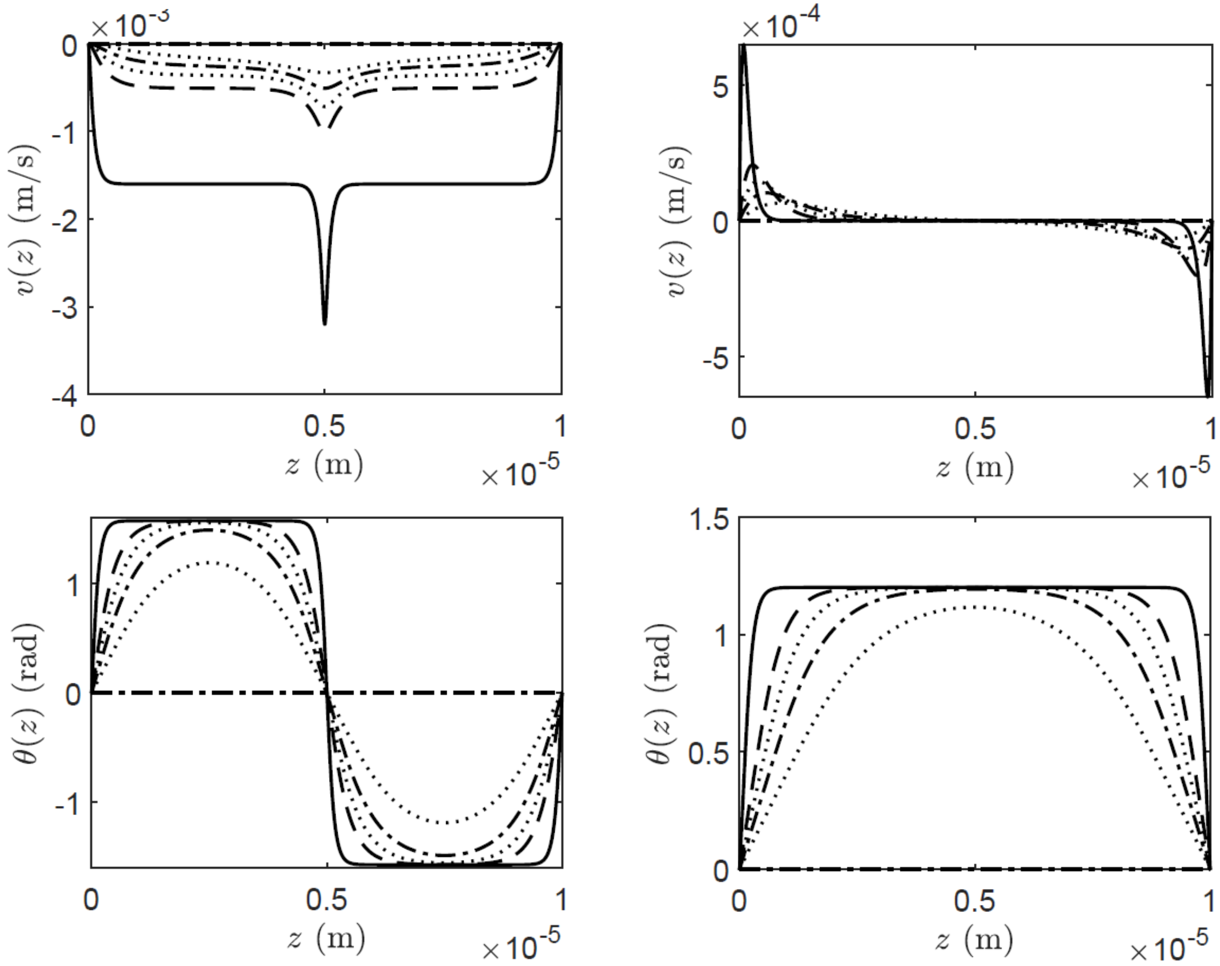


stable solutions have + or - mass flux

(but which one is chosen?)

Equilibrium solutions

- What about for $\zeta > 0$ (we already know that $\theta \equiv 0$ is stable)
- Are there non-trivial solutions? **(Yes…we find lots of solutions)**



symmetric flow

antisymmetric flow

antisymmetric director

symmetric director

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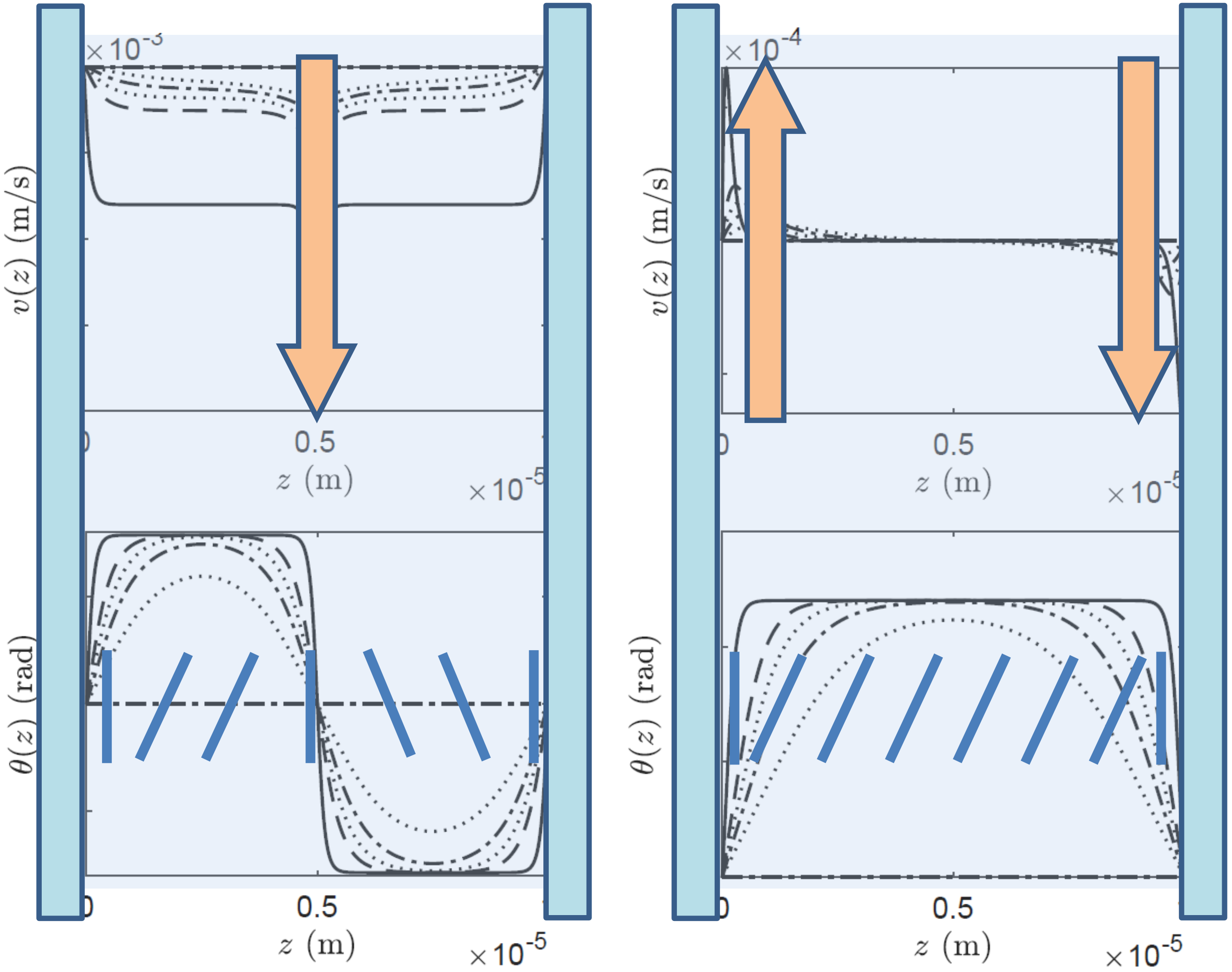


symmetric flow

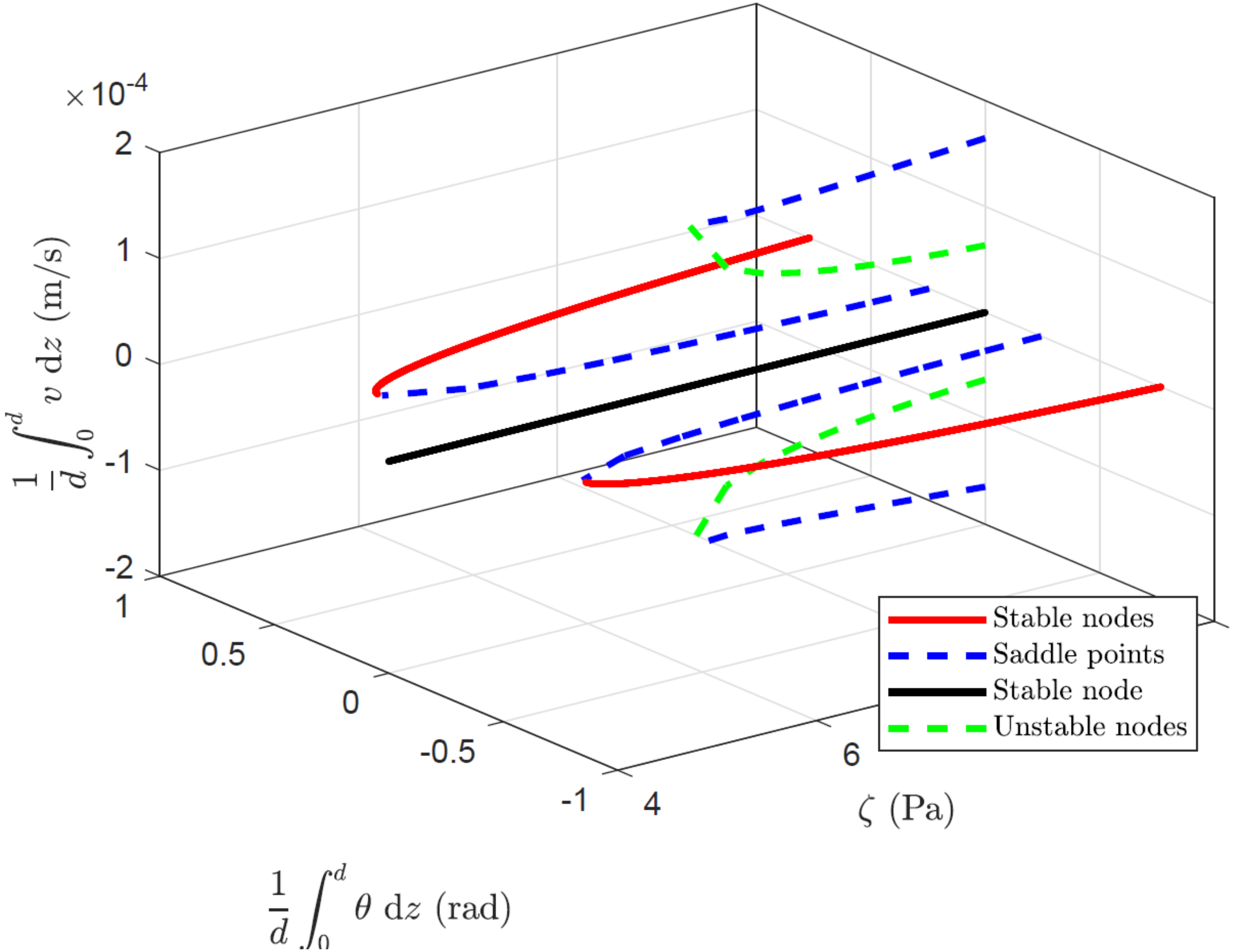
antisymmetric director

antisymmetric flow

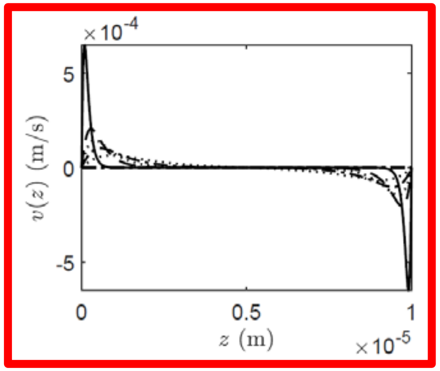
symmetric director

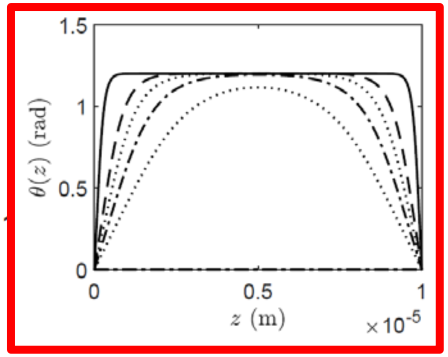
Equilibrium solutions

- For pullers (ζ >0) the non-trivial solutions are not connected to the trivial branch



trivial solution is global minimiser

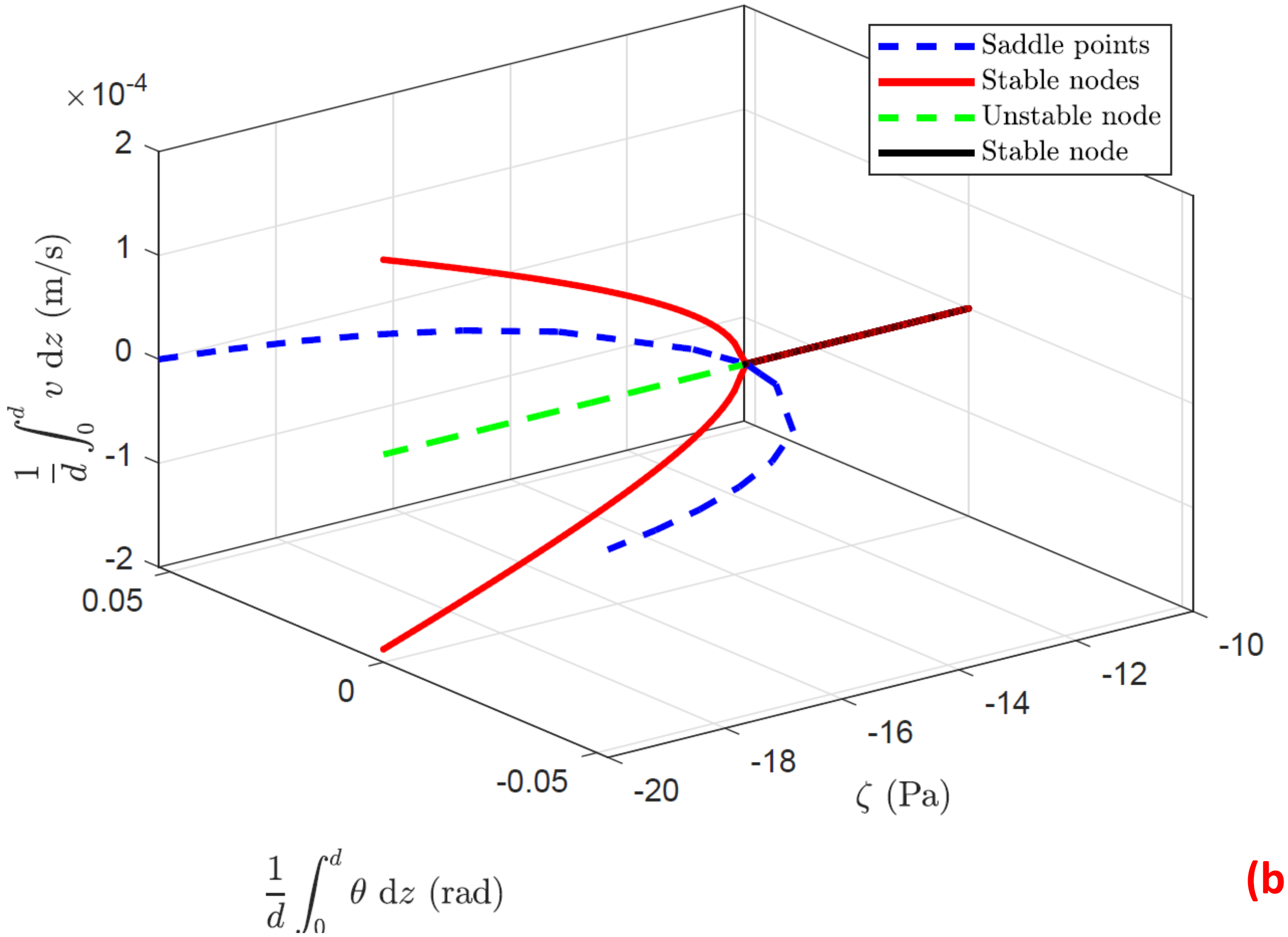


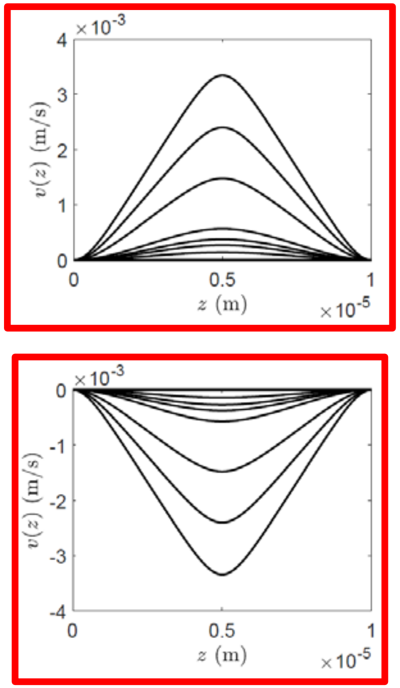


stable solution has zero mass flux

Designing active flows

- We imagine that we wish the active material to self-propel
- Can we chose a particular stable state?



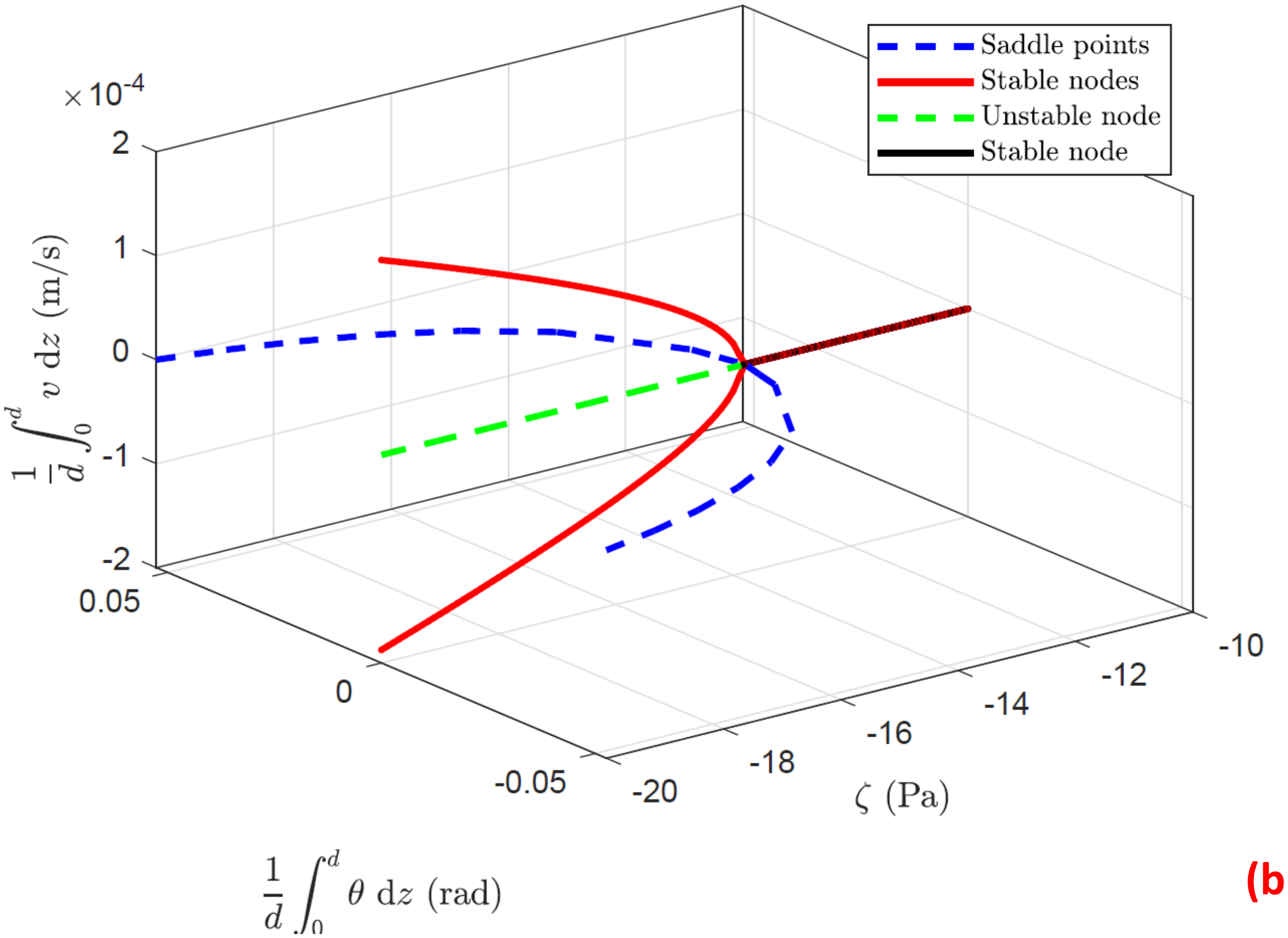


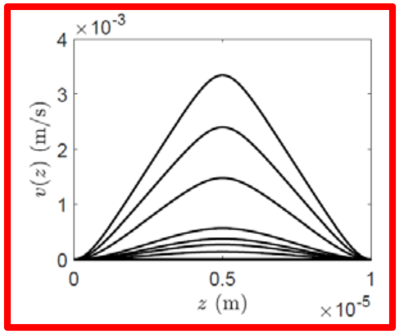
stable solution have + or - mass flux

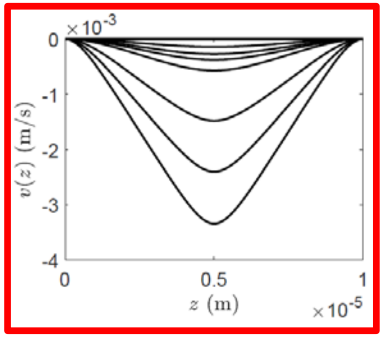
(but which one is chosen?)

Designing active flows

- Yes we can…we apply a pressure gradient and one of the states is preferred…







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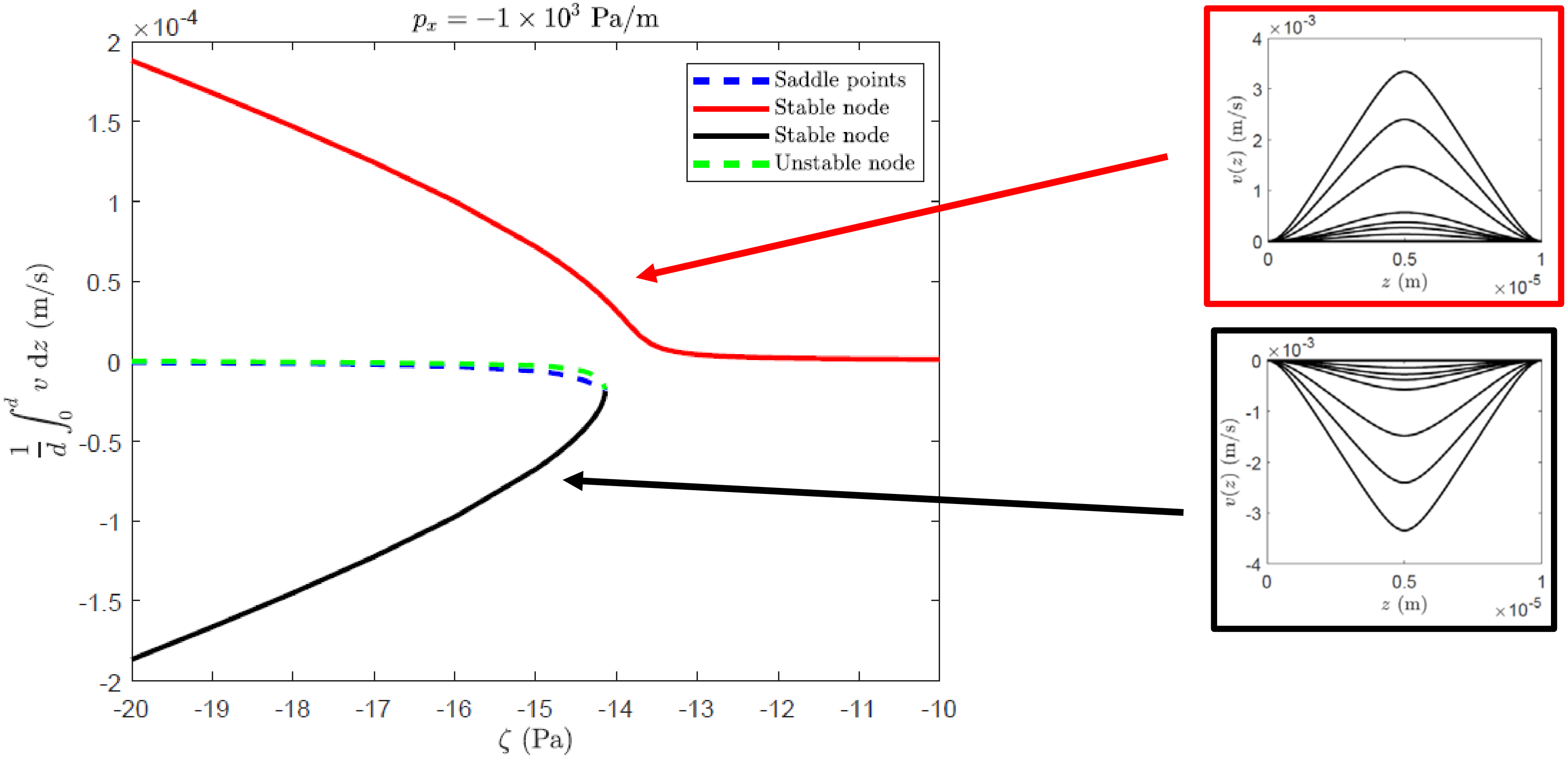
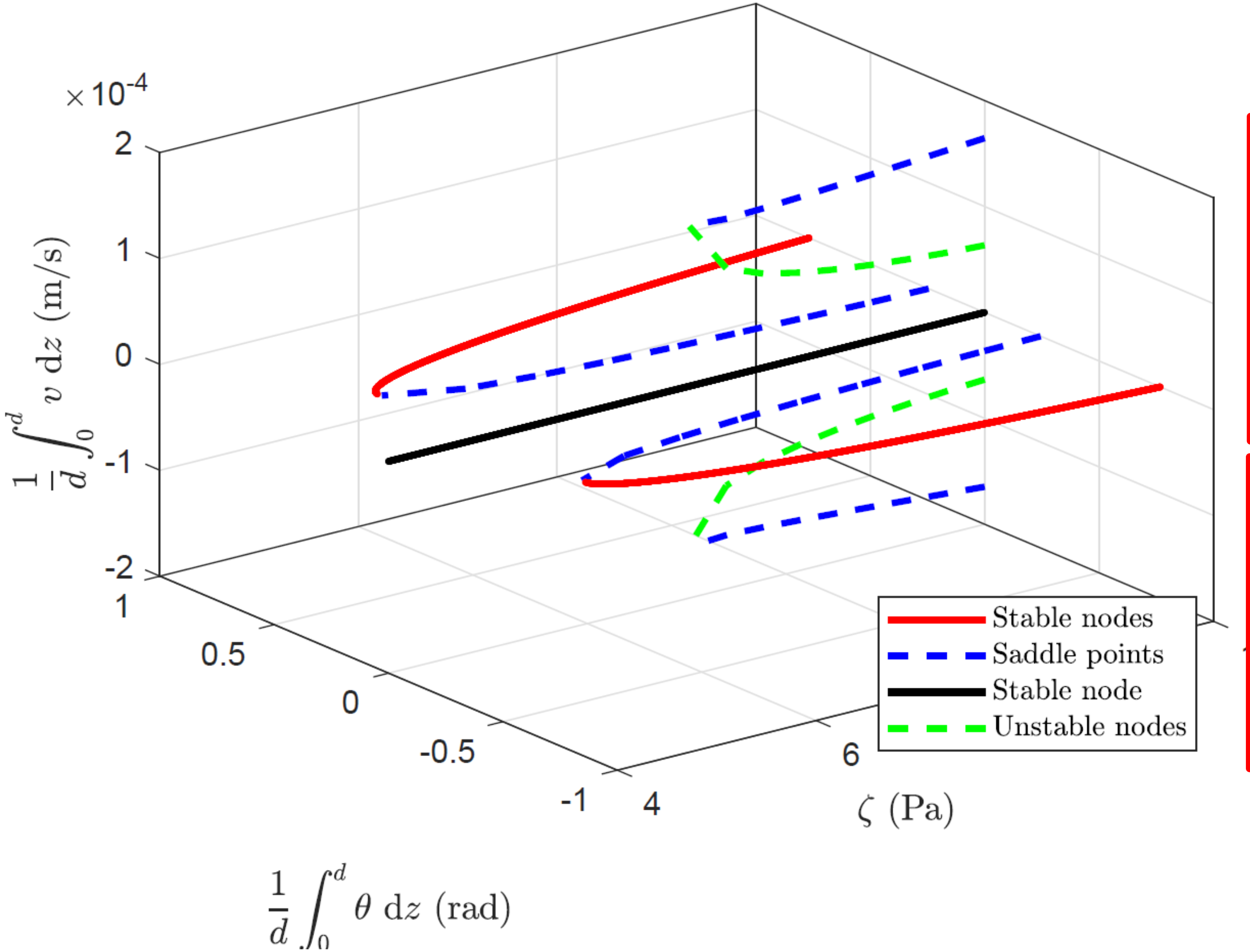
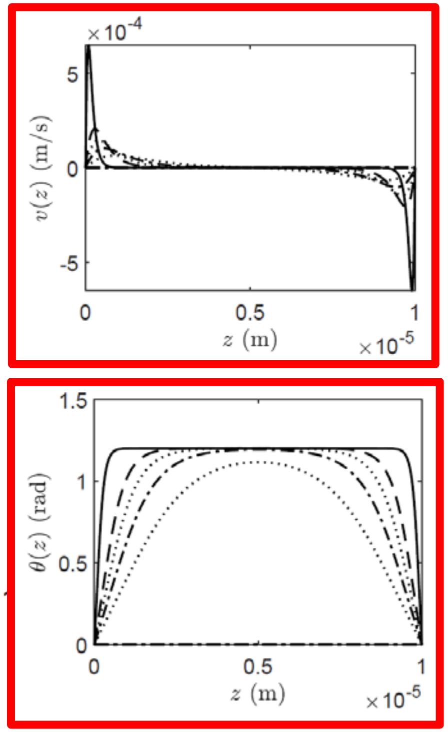


Designing active flows

- What about pullers (ζ>0)… can we access the metastable state?



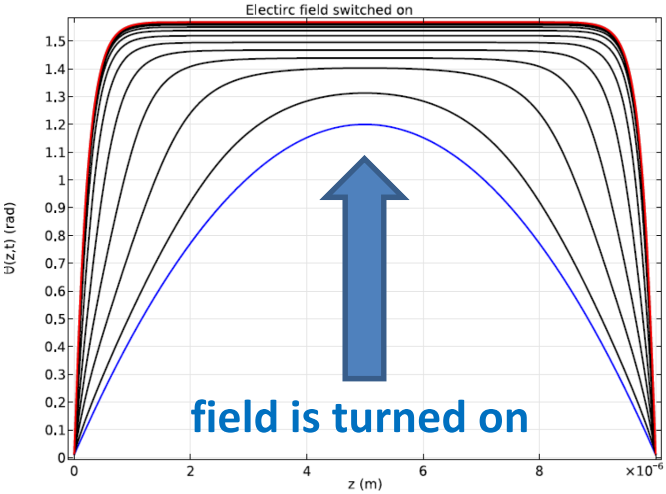
trivial solution is global minimiser

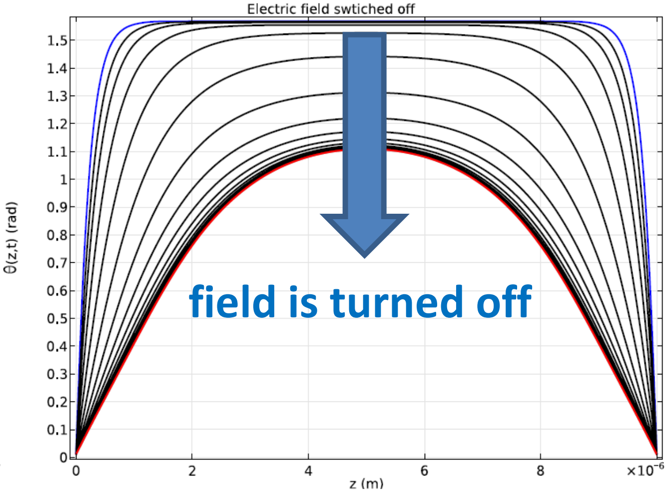


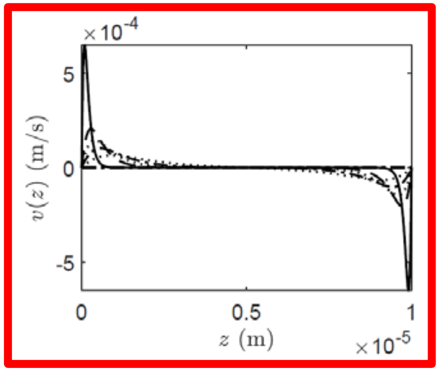
Designing active flows

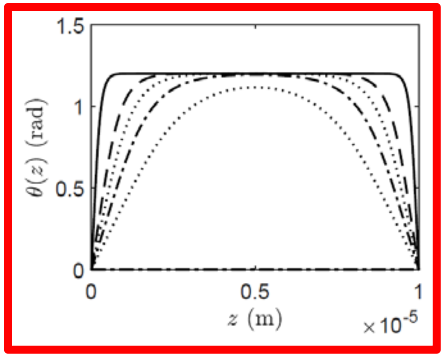
- What about pullers (ζ>0)… can we access the metastable state?
- Yes…with **pretilt and an external orienting field**

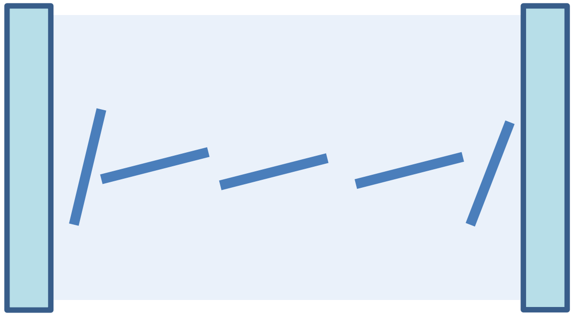
trivial solution is global minimiser





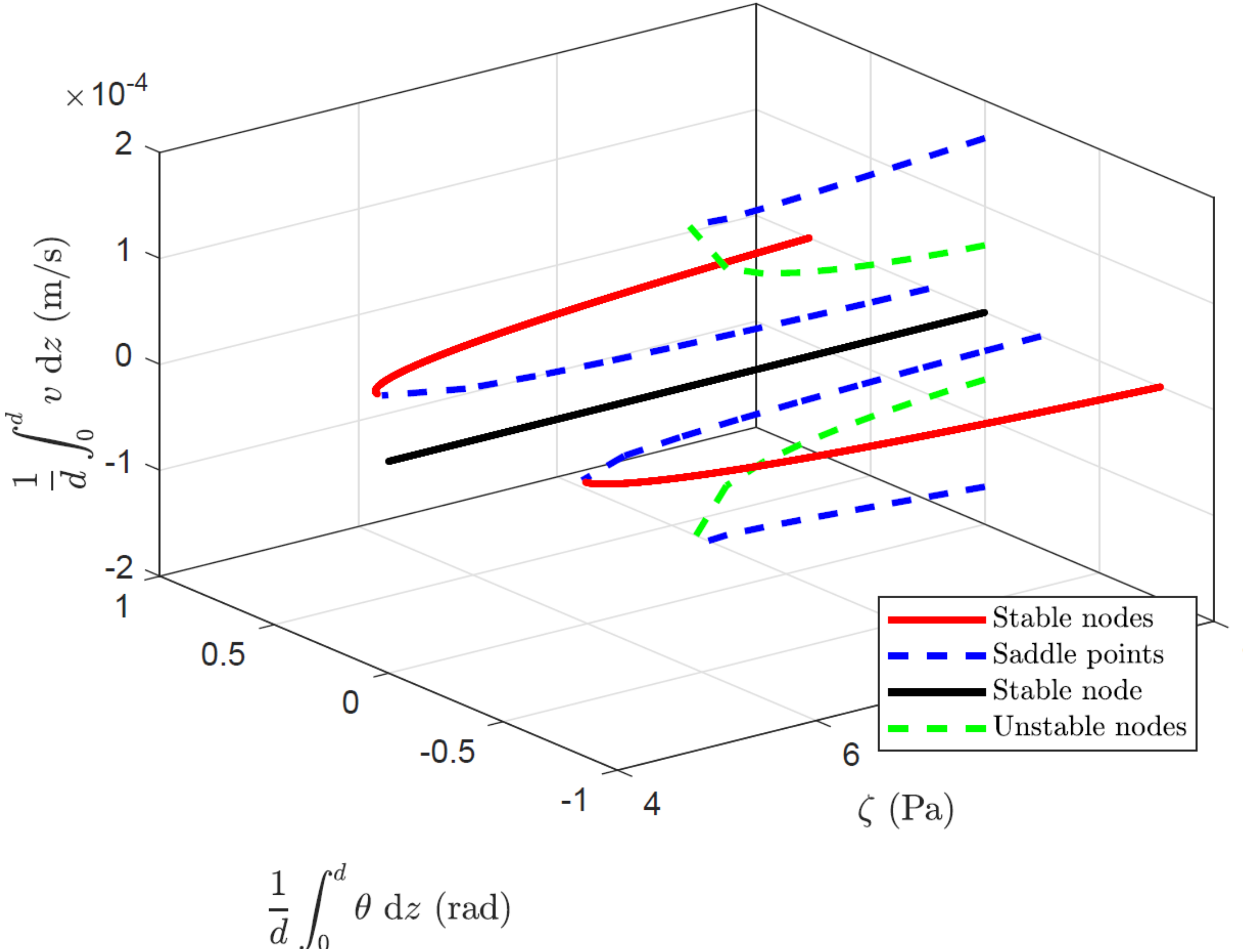


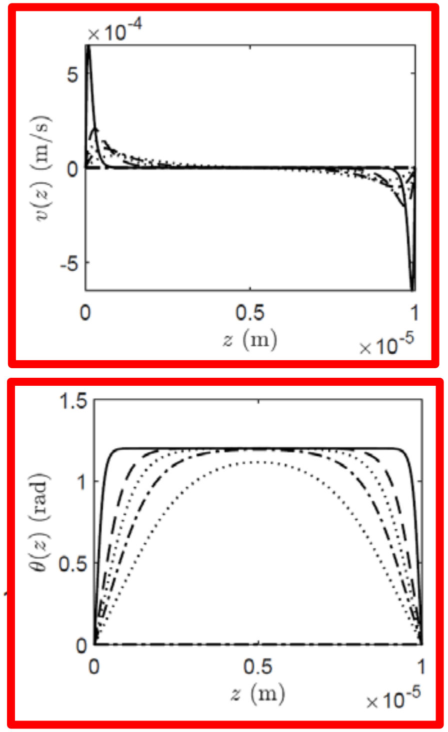




Designing active flows

- Could we access the saddle point solutions (even though they are unstable)?





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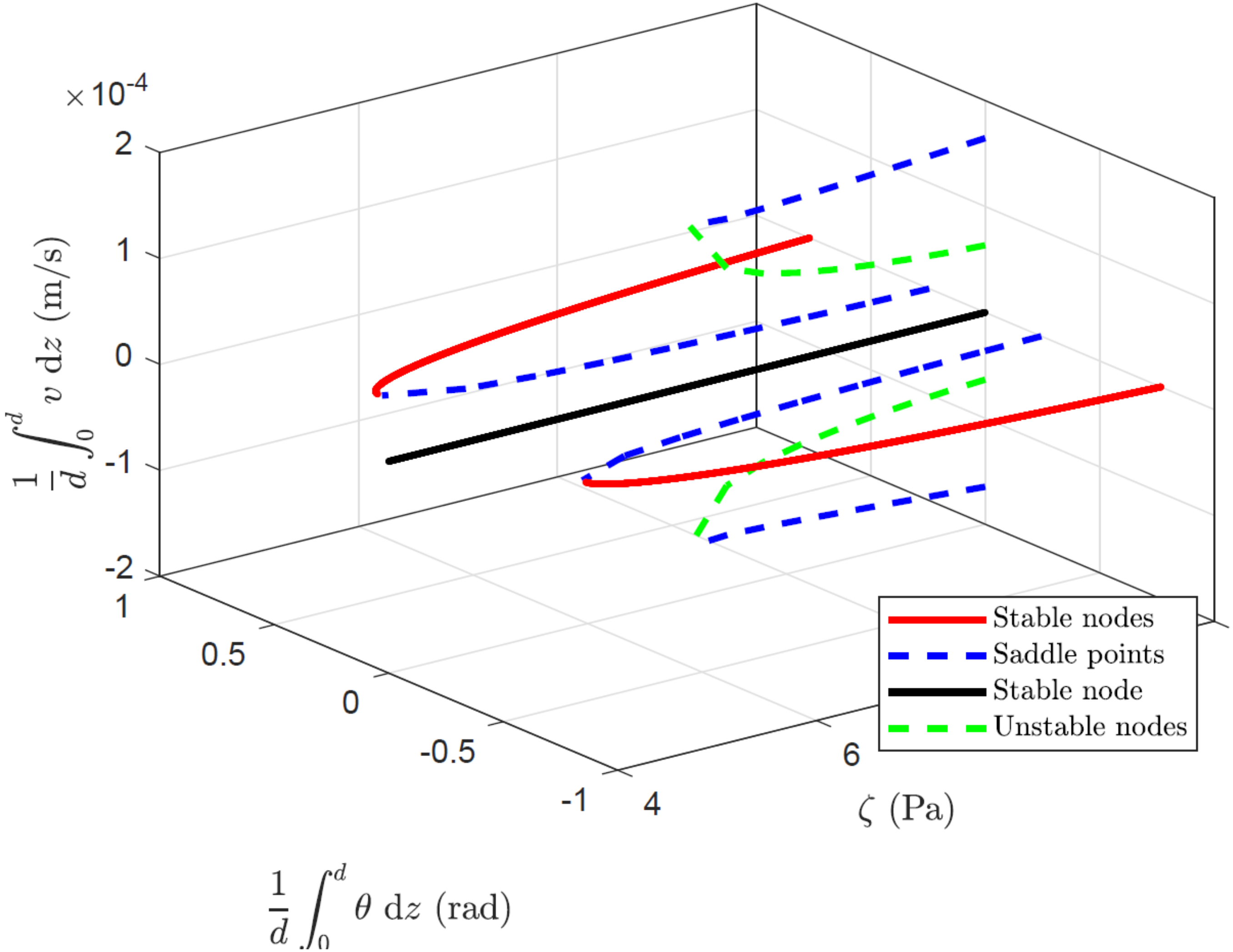
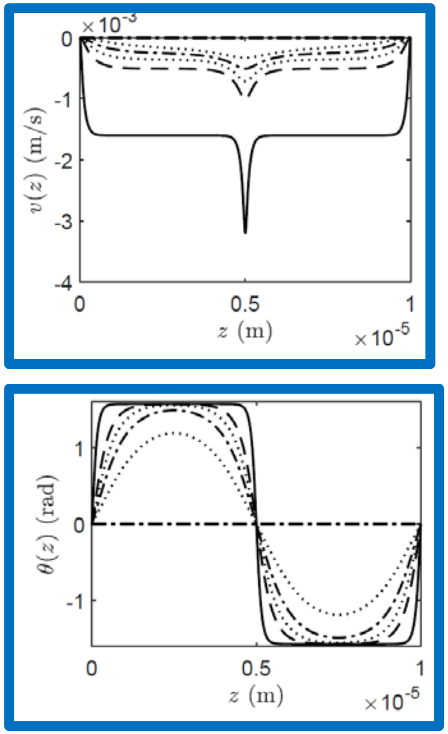


jet flow



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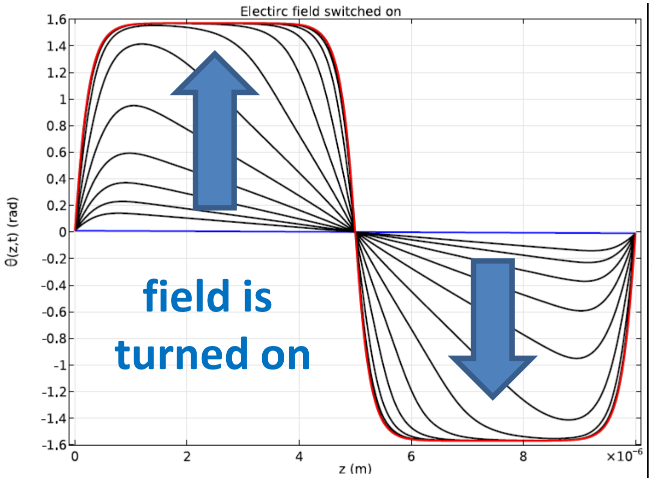
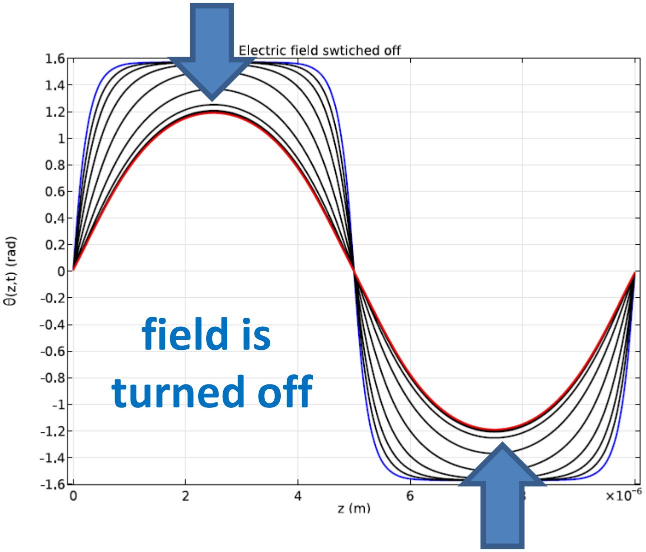
- Could we access the saddle point solutions (even though they are unstable)?

- Yes…again with **pretilt and an external orienting field**



field is turned on



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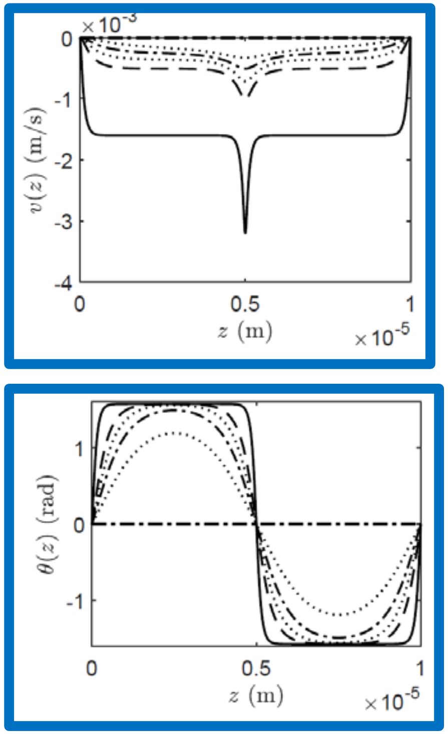
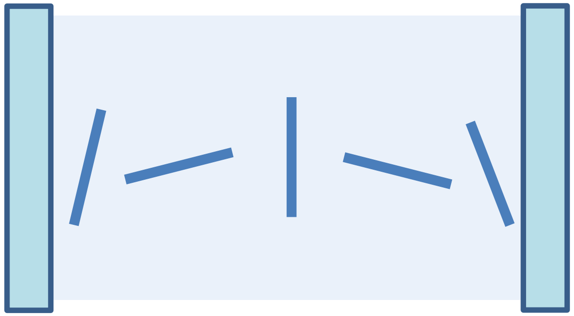
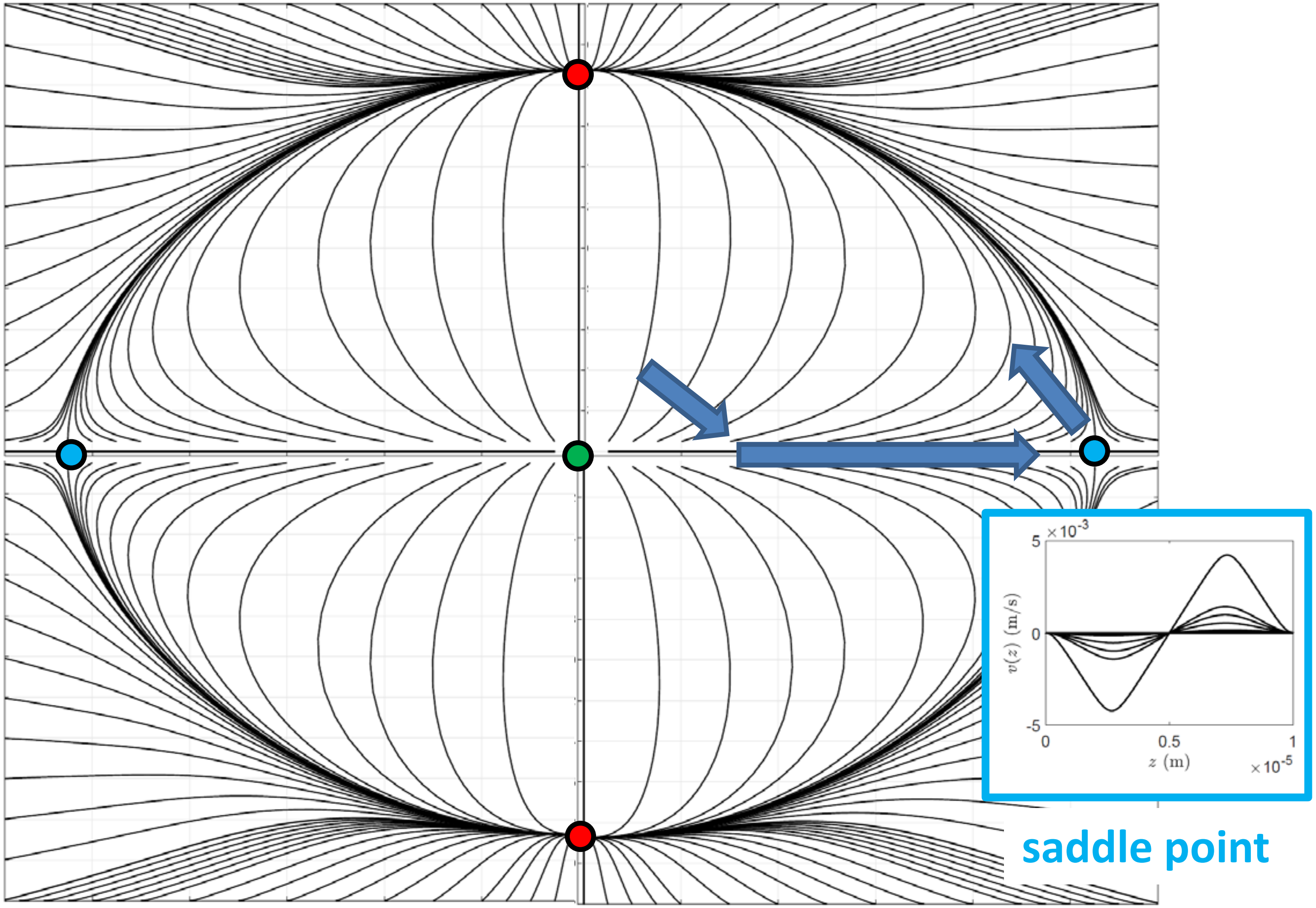




Designing active flows

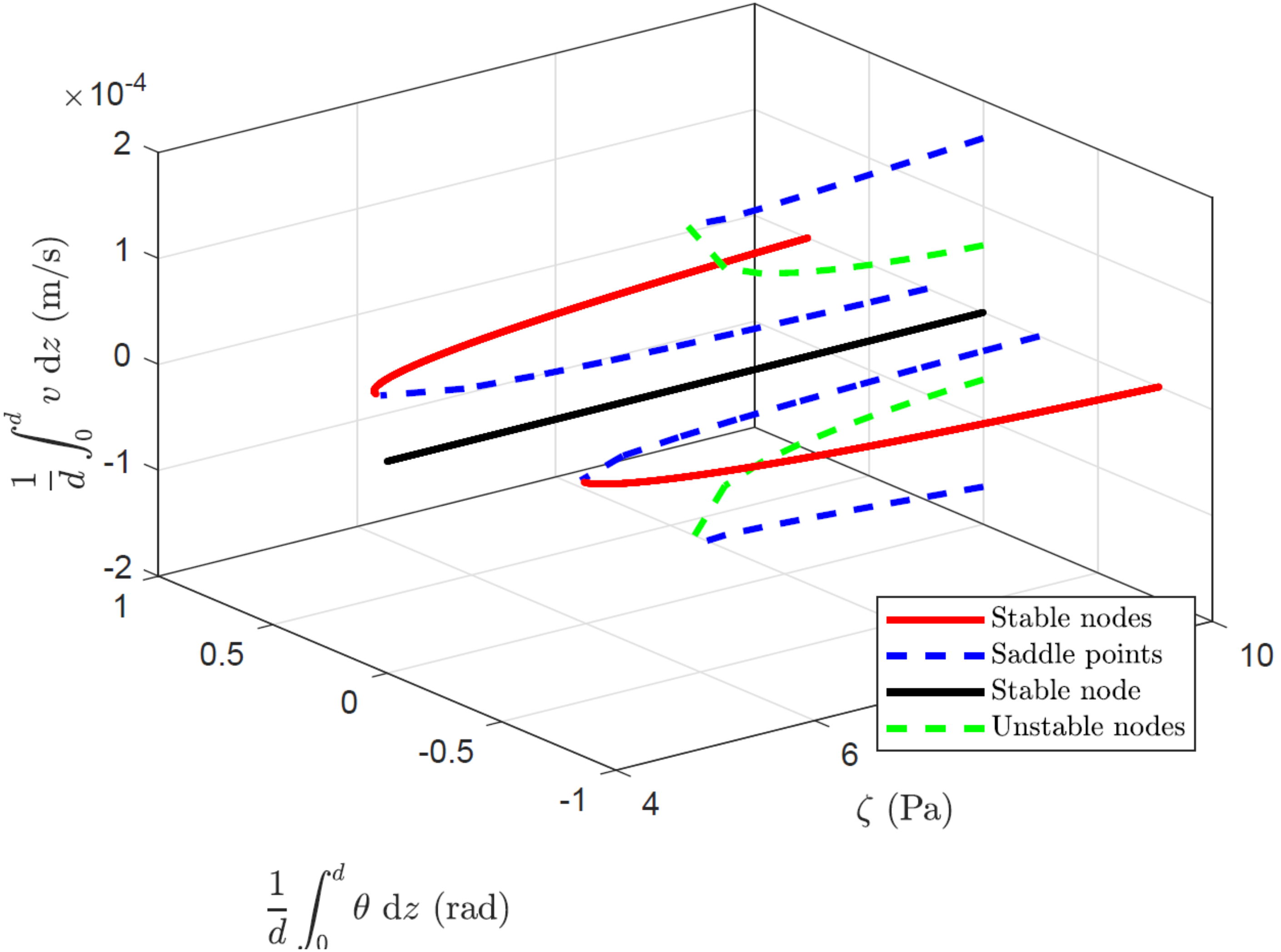
- We can map trajectories of the system in terms of two measures



saddle point

Designing active flows

- What does an applied pressure do to our puller solutions (ζ>0)?



Designing active flows

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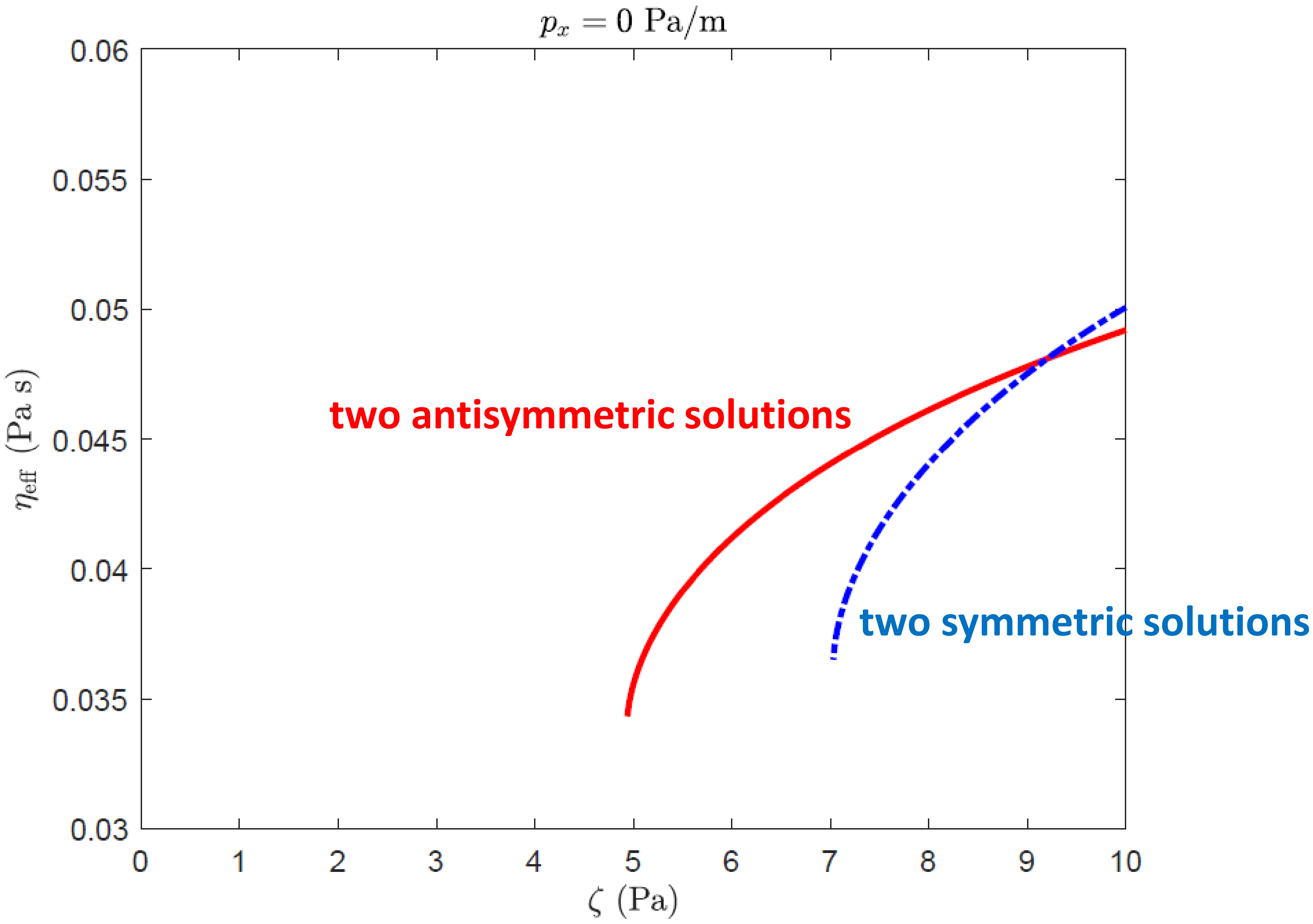

Designing active flows

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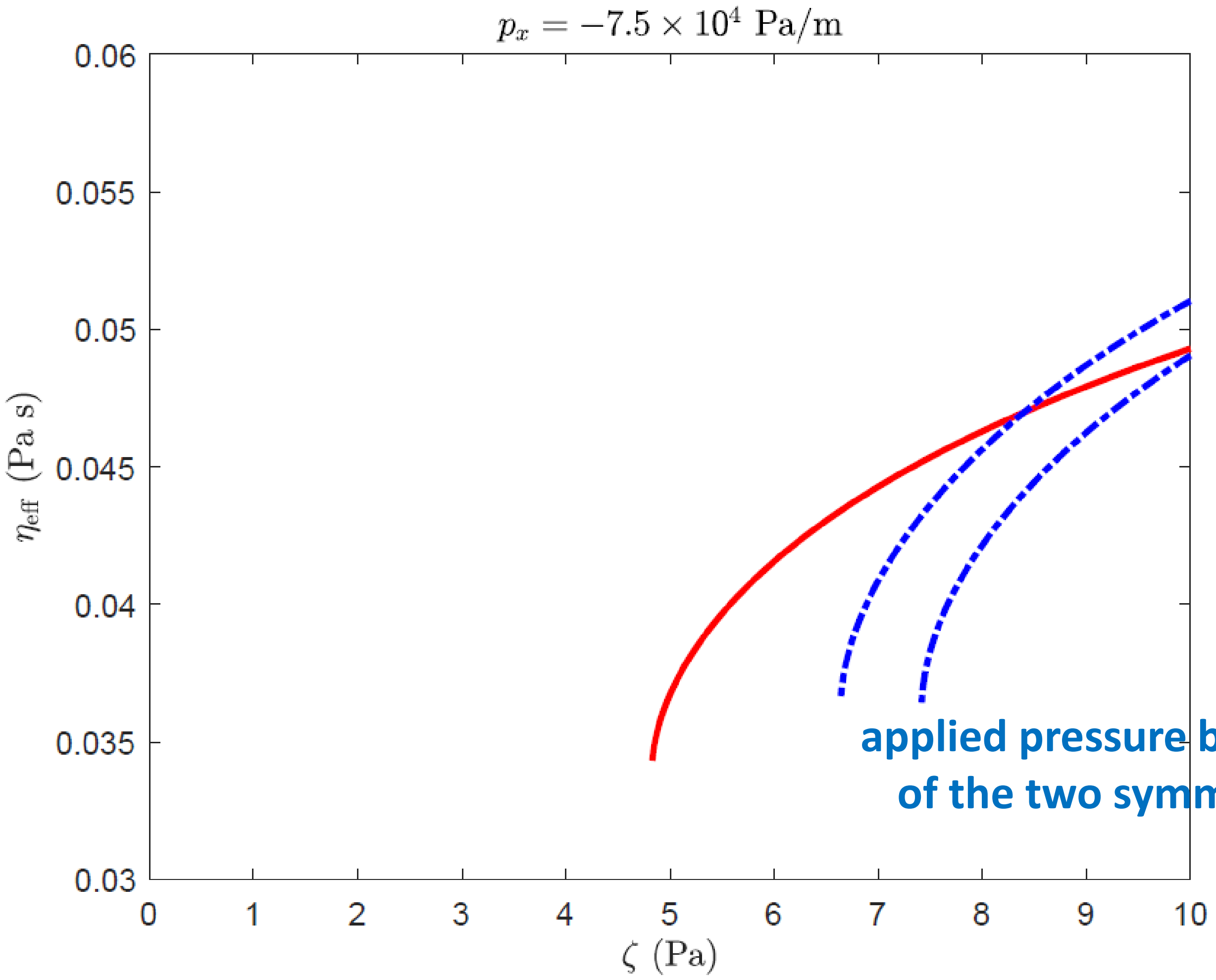
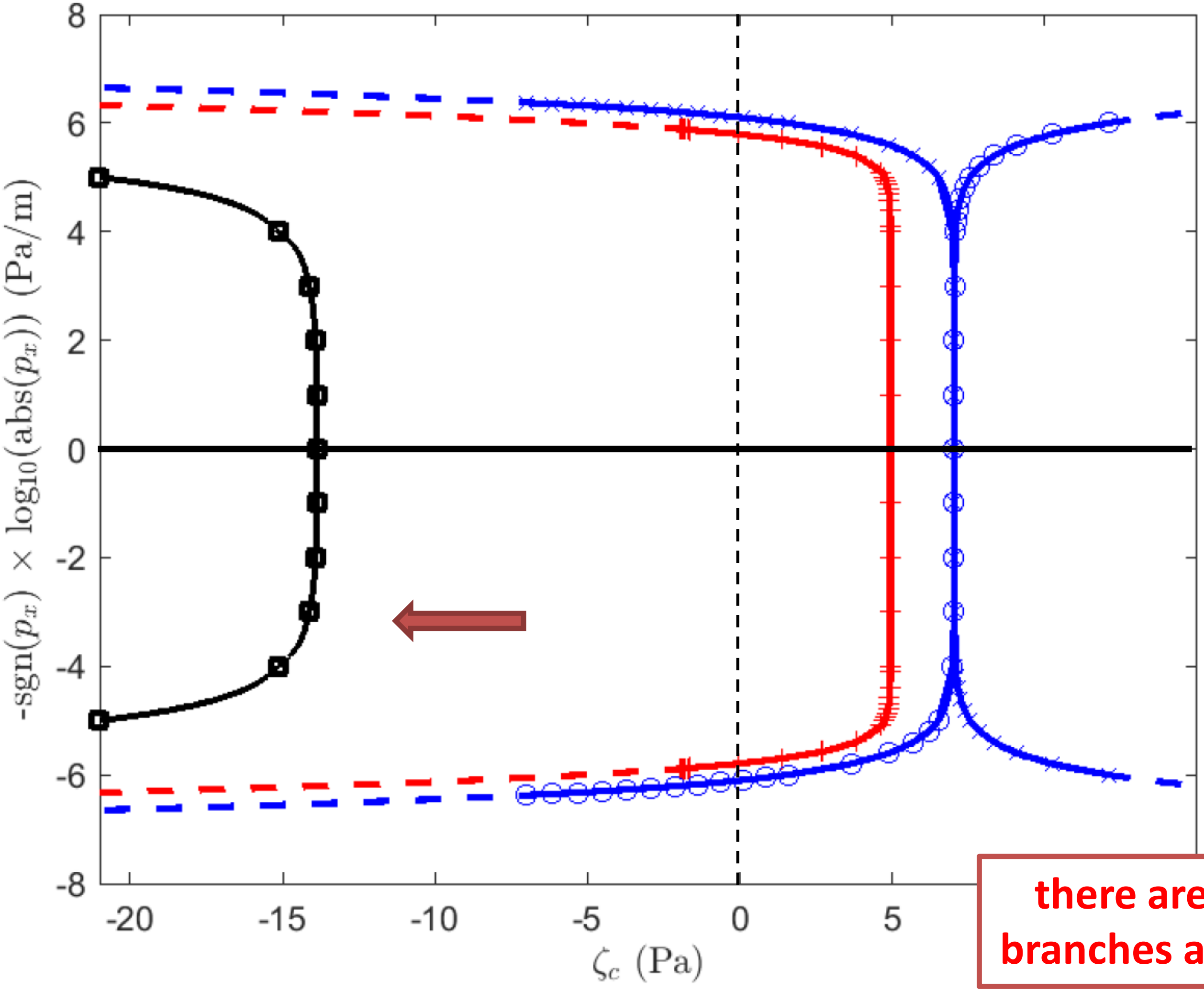


applied pressure breaks symmetry of the two symmetric solutions

Designing active flows

- What does an applied pressure do to our puller solutions (ζ>0)?

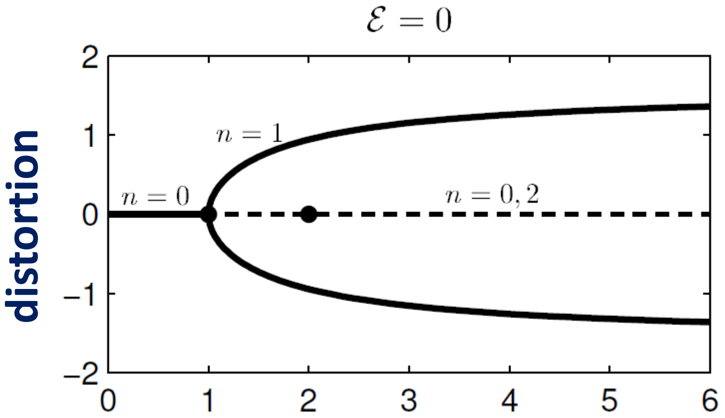


there are non-trivial branches at zero activity

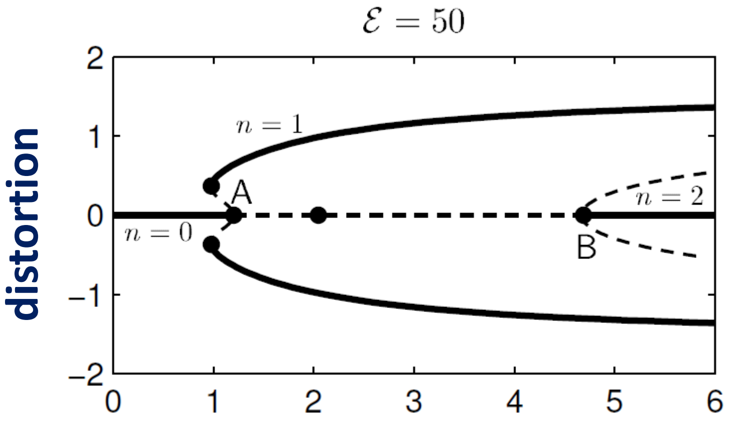
Inactive flows in an electric field

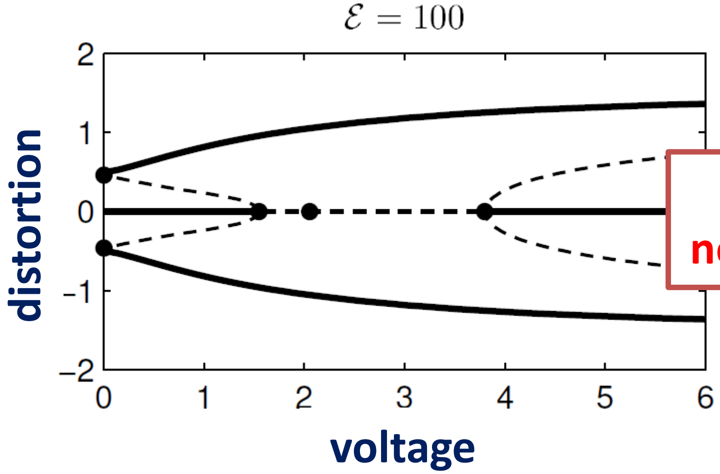
- Classic Freedericksz cell: an applied pressure gradient can perturb the system and lead to non-trivial solutions at zero electric field

no applied pressure:
classic Freedericksz transition



intermediate pressure:
perturbed pitchfork bifurcation

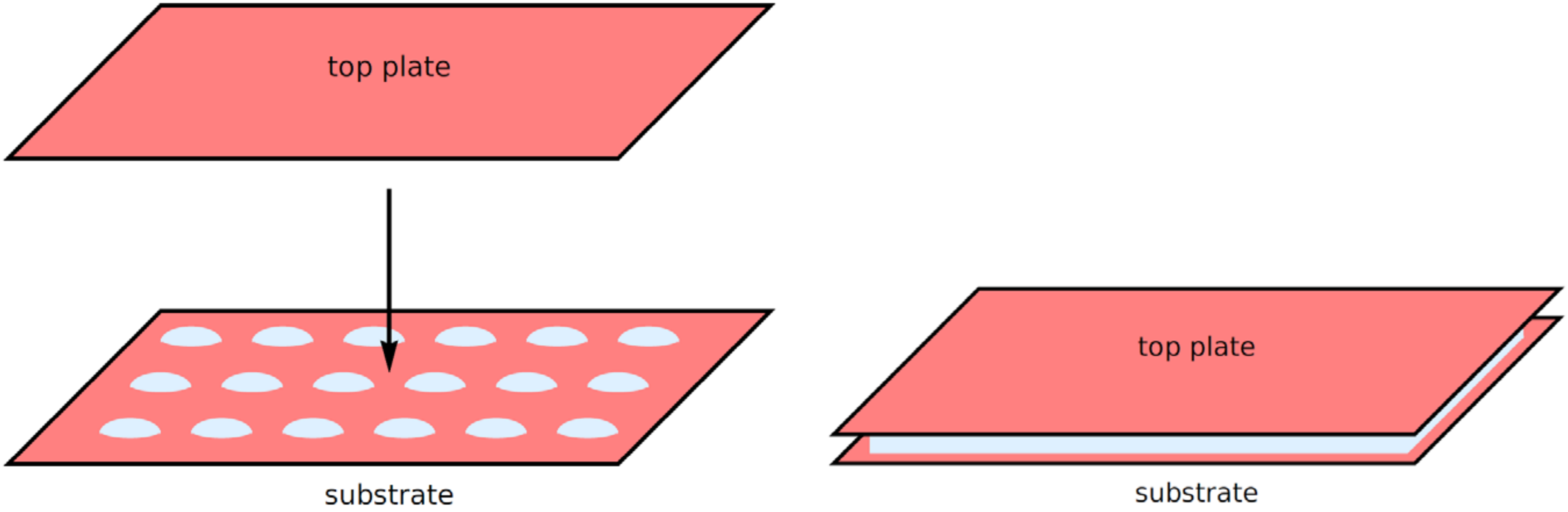




high pressure:
non-trivial branches at V=0

Flow during device filling

- The “one-drop-filling” method is regularly used by device manufacturers



- **But causes misalignment at the surface, leading to defects**

Flow during device filling

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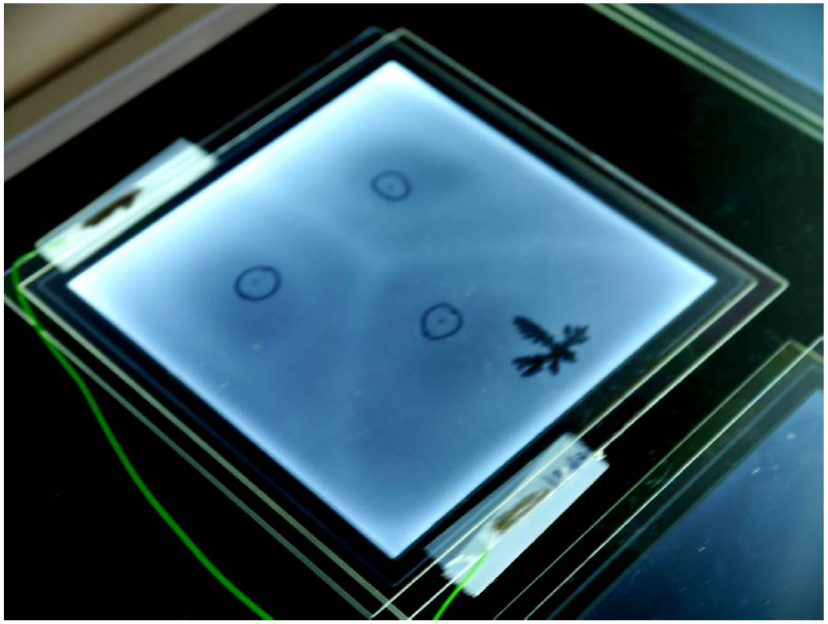

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Flow during device filling

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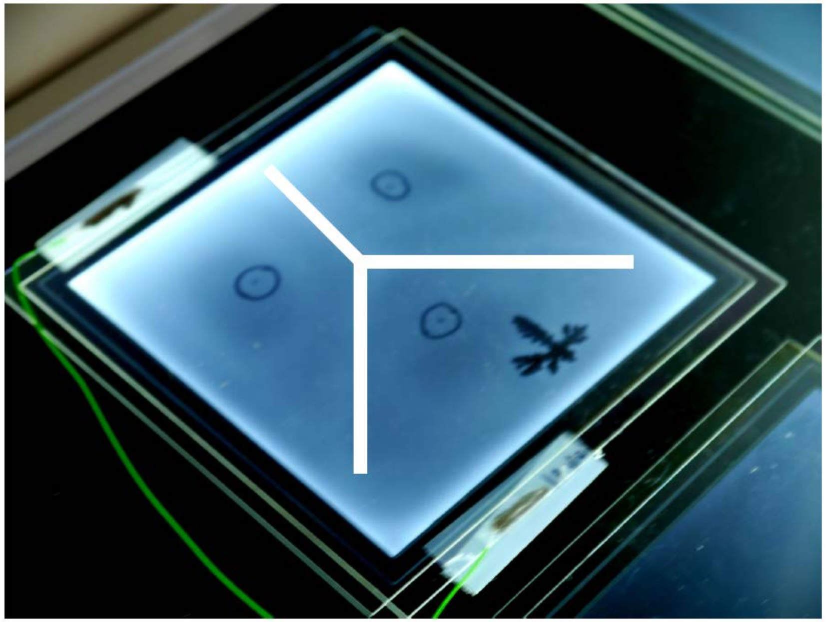
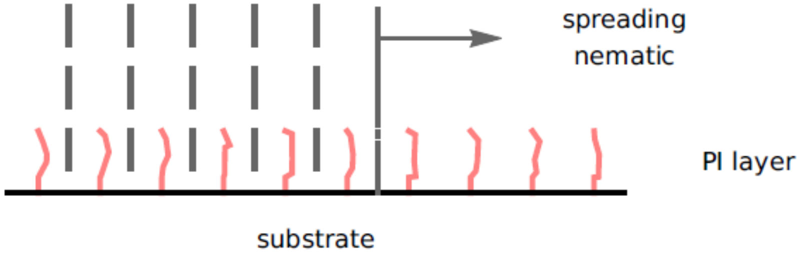
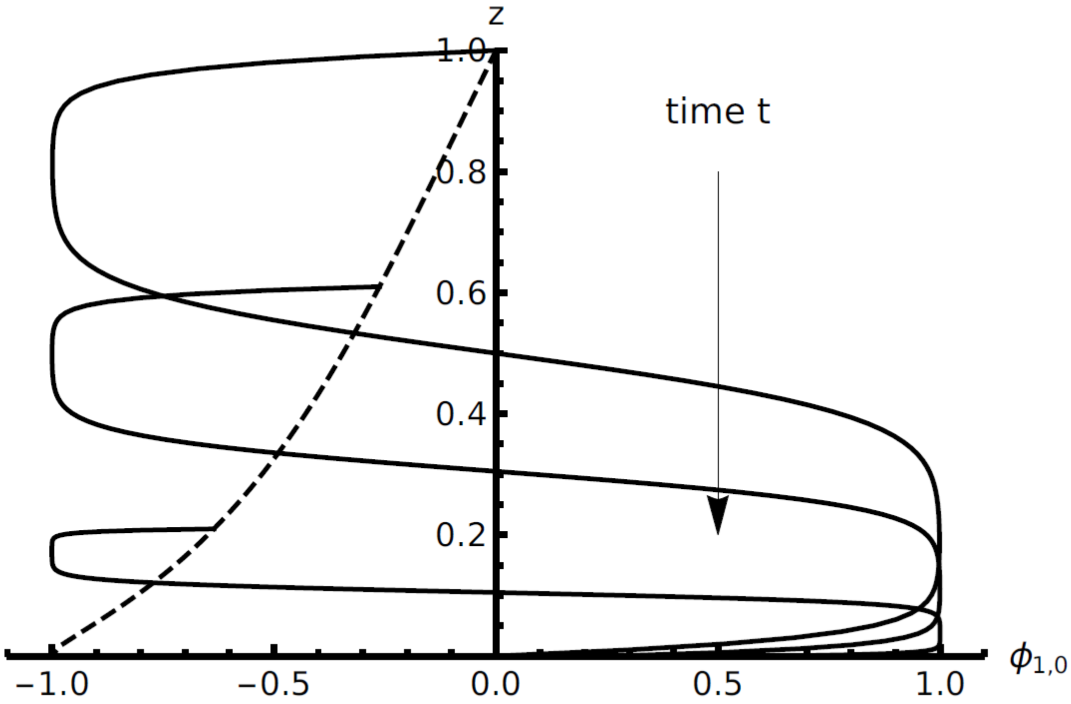




- **But causes misalignment at the surface, leading to defects**

Flow during device filling

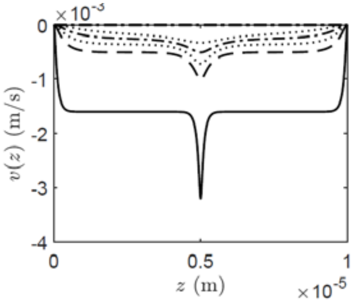
- Shear gradients at the substrates lead to the surface director being misaligned…**and surface dissipation could play a role**



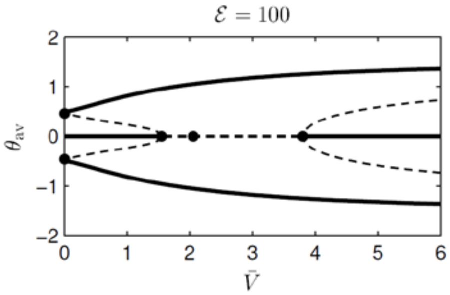
$$\underbrace{\gamma_S \frac{D\phi}{Dt}}_{\text{surface dissipation}} = \underbrace{K\frac{\partial\phi}{\partial z} - A\sin(2\phi)}_{\text{classical weak anchoring terms}}.$$

Rheology of active and inactive liquid crystals

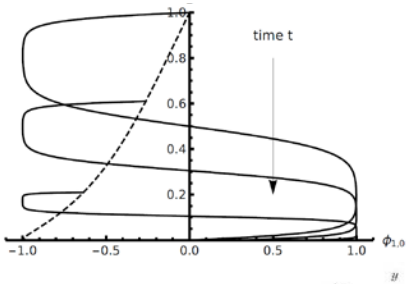
- Active liquid crystals:
  - **symmetric/antisymmetric solution branches, jet-like flow solutions**
  - **applied pressure breaks symmetry and prefers specific modes**



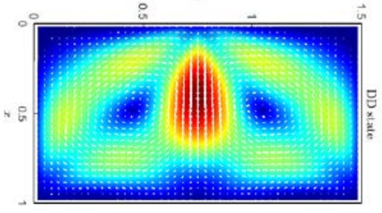
- Inactive liquid crystals:
  - **applied pressure can produce non-trivial states without extra forcing**



- Squeeze-film flows:
  - **high shear leads to damage to substrate orientation**



- 2-dimensions:
  - **how will various streamwise modes interact with cross –sectional structures?**



Rheology of active and inactive liquid crystals

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