Lecture 2: Numerical Methods for Hopf bifurcations and periodic orbits in large systems

Alastair Spence

Department of Mathematical Sciences
University of Bath

CLAPDE, Durham, July 2008

1. Introduction
2. Calculation of Hopf points
3. Hopf detection using bifurcation theory
4. Hopf detection using Complex Analysis
5. Hopf detection using the Cayley Transform
6. Stable and unstable periodic orbits

Outline

1. Introduction
2. Calculation of Hopf points
3. Hopf detection using bifurcation theory
4. Hopf detection using Complex Analysis
5. Hopf detection using the Cayley Transform
6. Stable and unstable periodic orbits

Recap and plan for today

- Lecture 1:
  1. Compute paths of $F(x, \lambda) = 0$ using pseudo-arclength
  2. Detect singular points $\mathrm{Det}(F_x(x, \lambda)) = 0$
  3. Compute paths of singular points in two-parameter problems
  4. bordered systems
  5. 4-6 cell interchange in the Taylor problem
- Lecture 2:
- Accurate calculation of Hopf points
- Detection of Hopf bifurcations (find pure imaginary eigenvalues in a large sparse parameter-dependent matrix)
  1. Bifurcation theory
  2. Complex analysis
  3. Cayley transform
- Stable and unstable periodic orbits

Lecture 1: Compute singular points

- Seek (x, λ) such that $F_x(x, \lambda)$ is singular
- Consider

$$\begin{bmatrix} F_x(x,\lambda) & F_\lambda(x,\lambda) \\ c^T & d \end{bmatrix} \begin{bmatrix} * \\ g \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

- $\mathrm{Det}(F_x) = 0 \iff g = 0$.
- Accurate calculation: Consider the pair

$$F(x,\lambda) = 0, \quad g(x,\lambda) = 0$$

- Newton's Method:

$$\begin{bmatrix} F_x(x,\lambda) & F_\lambda(x,\lambda) \\ g_x(x,\lambda)^T & g_\lambda(x,\lambda) \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta \lambda \end{bmatrix} = - \begin{bmatrix} F \\ g \end{bmatrix}$$

- System nonsingular if $\frac{d}{dt}\mu \neq 0$ at singular point

Outline

1. Introduction
2. Calculation of Hopf points
3. Hopf detection using bifurcation theory
4. Hopf detection using Complex Analysis
5. Hopf detection using the Cayley Transform
6. Stable and unstable periodic orbits

Accurate calculation of Hopf points

- Assume $A(\lambda) = F_x(x, \lambda)$ is real and nonsingular
- At Hopf point: $A(\lambda)$ has eigenvalues $\pm i\omega$
- $\mathrm{Rank}(A(\lambda)^2 + \omega^2 I) = n - 2$

Accurate calculation of Hopf points

- Assume $A(\lambda) = F_x(x,\lambda)$ is real and nonsingular
- At Hopf point: $A(\lambda)$ has eigenvalues $\pm i\omega$
- $\text{Rank}(A(\lambda)^2 + \omega^2 I) = n - 2$
- Calculate Hopf point using 2-bordered matrix: set up

$$F(x,\lambda) = 0, \quad g(x,\lambda,\omega) = 0, \quad h(x,\lambda,\omega) = 0$$

where

$$\begin{bmatrix} A(\lambda)^2 + \omega^2 I & B \\ C^T & D \end{bmatrix} \begin{bmatrix} * \\ g \\ h \end{bmatrix} = \begin{bmatrix} 0 \\ r_1 \\ r_2 \end{bmatrix}$$

- Newton system, $(n+2) \times (n+2)$, needs $g_x, g_\lambda, g_\omega, h_x, \ldots$
- Block version of (D)+iterative refinement on (C)
- 2-bordered matrix is nonsingular if complex pair cross imaginary axis “smoothly”

Hopf continued

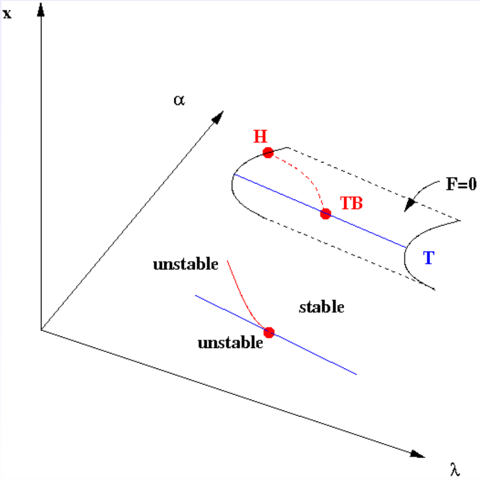
- $A(\lambda) = F_x(x, \lambda)$
- If you don't want to form $A(\lambda)^2$: split complex eigenvector/eigenvalue into Real and Imaginary parts and work with $(2n+2) \times (2n+2)$ matrices involving $A(\lambda)$
- Extensions for N-S: $A(\lambda)\phi = \mu B \phi$
- BUT: Whatever system is used, accurate estimates for λ and ω are needed
- Compute paths of Hopf points in 2-parameter problems (3-bordered matrices)
- Summary of methods: Govaerts (2000)

Outline

1. Introduction
2. Calculation of Hopf points
3. Hopf detection using bifurcation theory
4. Hopf detection using Complex Analysis
5. Hopf detection using the Cayley Transform
6. Stable and unstable periodic orbits

Bifurcation Theory: Takens-Bogdanov (TB) point

At a TB point, F_x has a 2-dim Jordan block, i.e. $\begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$. A typical picture is:



"Organising Centre" Algorithm

- Two parameter problem $F(x, \lambda, \alpha) = 0$
- Fix α. Compute a Turning point in (x, λ)(Easy!). Remember:

$$F_x \phi = 0, \quad (F_x)^T \psi = 0$$

- For the 2-parameter problem: Compute path of Turning points looking for $\psi^T \phi = 0$ (TB point) (Easy)
- Jump onto path of Hopf points (symmetry-breaking) (Easy)
- Compute path of Hopf points (pseudo-arclength) (Easy)
- In parameter space the paths of Hopf and Turning points are tangential at TB

5 cell anomalous flows in the Taylor Problem

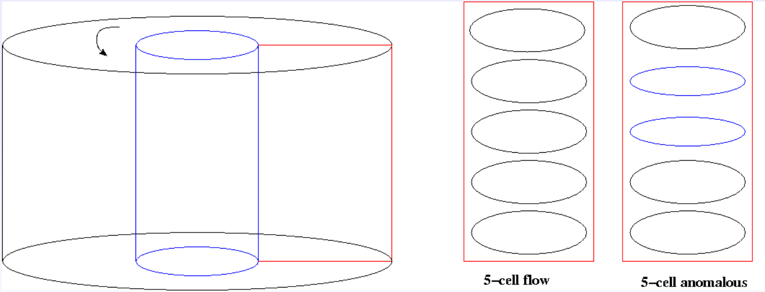


Figure: Two different 5-cell flows

5-cell flows experimental results

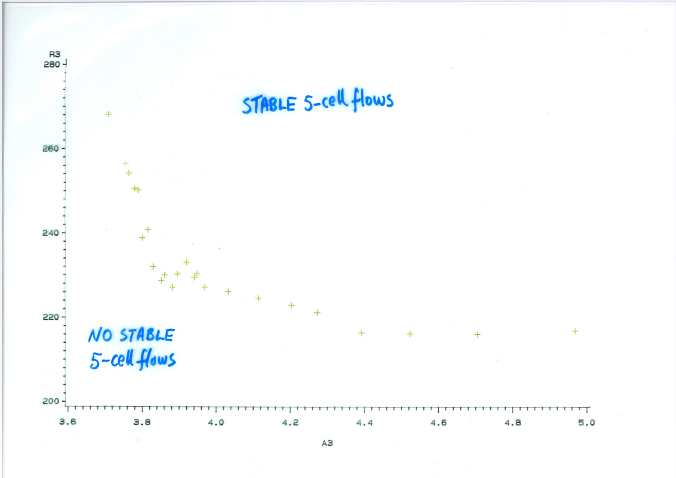


Figure: parameter space plots of 5-cell flows

5-cell flows numerical results (Anson)

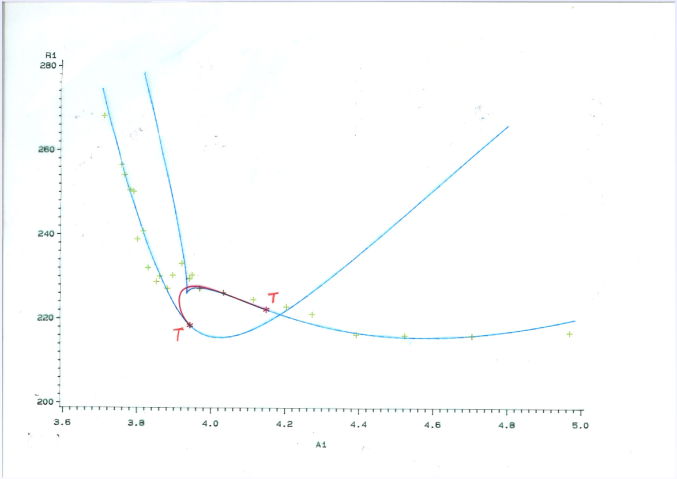


Figure: parameter space plots of 5-cell flows

"Organising Centre" approach

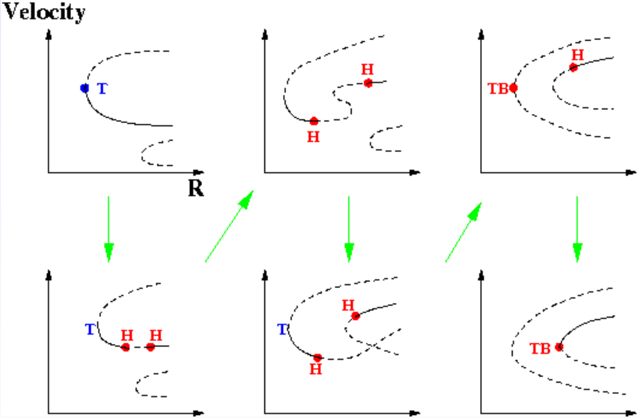


Figure: 5-cell flows: Sequence of Bifurcation diagrams as aspect ratio changes

This understanding wouldn't be possible without the numerical results

Outline

1 Introduction

2 Calculation of Hopf points

3 Hopf detection using bifurcation theory

4 Hopf detection using Complex Analysis

5 Hopf detection using the Cayley Transform

6 Stable and unstable periodic orbits

The "idea": Govaerts/Spence (1996)

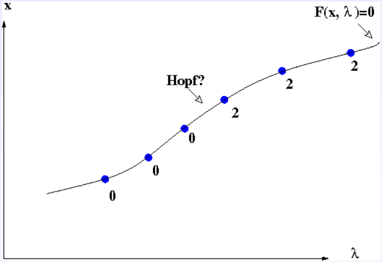


Figure: For each point on $F(x, \lambda) = 0$ can we calculate the **number** of eigenvalues in the unstable half plane?

Why Nice?

(a) Seek an integer, and (b) Estimate for $\mathrm{Im}(\mu)$ not needed.

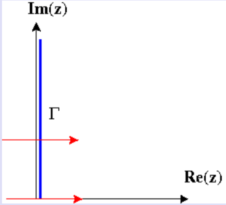
Complex Analysis

Winding number

If $g(z)$ is analytic in Γ

$$\begin{aligned} N - P &= \frac{1}{2\pi}[\arg g(z)]_\Gamma \\ &= \text{Winding Number} \\ &= W(g) \end{aligned}$$

Contour for real matrices



Algorithm

- "Counting Sectors": Ying/Katz (1988) (based on Henrici (1974))

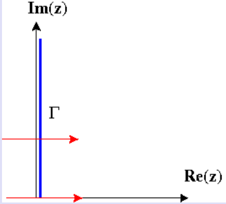
Complex Analysis

Winding number

If $g(z)$ is analytic in Γ

$$\begin{aligned} N - P &= \frac{1}{2\pi}[\arg g(z)]_\Gamma \\ &= \text{Winding Number} \\ &= W(g) \end{aligned}$$

Contour for real matrices



Algorithm

- "Counting Sectors": Ying/Katz (1988) (based on Henrici (1974))
- If g changes so that a real pole crosses Left to Right, $W(g)$ decreases by π. (real zero crosses L to R then $W(g)$ increases)
- If g changes so that a complex pole crosses Left to Right, $W(g)$ decreases by 2π

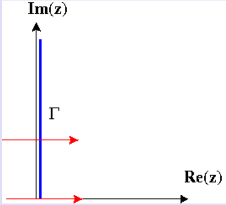
Complex Analysis

Winding number

If $g(z)$ is analytic in Γ

$$\begin{aligned} N - P &= \frac{1}{2\pi}[\arg g(z)]_\Gamma \\ &= \text{Winding Number} \\ &= W(g) \end{aligned}$$

Contour for real matrices



Algorithm

- “Counting Sectors”: Ying/Katz (1988) (based on Henrici (1974))
- If g changes so that a real pole crosses Left to Right, $W(g)$ decreases by π. (real zero crosses L to R then $W(g)$ increases)
- If g changes so that a complex pole crosses Left to Right, $W(g)$ decreases by 2π
- Need to evaluate $g(iy))$ on Γ

How to choose $g(z)$?

- Don't choose $g(z) = \mathrm{Det}(A(\lambda) - zI)$
- $\boxed{g(z) = c^T (A(\lambda) - zI)^{-1} b}$
- Schur complement of $M = \begin{bmatrix} A(\lambda) - zI & b \\ c^T & 0 \end{bmatrix}$
- poles are eigenvalues of $A(\lambda)$; zeros depend on choices of b and c. Choose b and c so that the zeros "cancel" the poles to keep $W(g)$ "small"
- Need to evaluate

$$g(iy) = c^T (A(\lambda) - iyI)^{-1} b$$

as y moves up Imaginary axis (Ying/Katz algorithm chooses y's)

The Tubular Reactor problem (Govaerts/Spence, 1996)

- Coupled pair of nonlinear parabolic PDEs for Temperature and Concentration
- Scaling: for a complex pole crossing Imag axis $W(g)$ reduces by 4

The Tubular Reactor problem (Govaerts/Spence, 1996)

- Coupled pair of nonlinear parabolic PDEs for Temperature and Concentration
- Scaling: for a complex pole crossing Imag axis $W(g)$ reduces by 4
- Winding numbers for 3 choices of g

point on path	$W(g_1)$	$W(g_2)$	$W(g_3)$
1	3	5	1
2	3	5	1
3	3	5	3^*
4	3	5	3
5	$-1^\dagger$	$1^\dagger$	$-1^\dagger$
6	-1	$3^\ddagger$	$1^\ddagger$

1. $^* =$ zero of g_3
2. $^\dagger =$ Hopf!
3. $^\ddagger =$ zero of g_2 and g_3.

Final comments on "Winding Number" algorithm

- Govaerts/Spence was "proof of concept": tested on a "not too difficult" problem
- Work is to evaluate

$$g(iy) = c^T (A(\lambda) - iyI)^{-1} b$$

  as y moves up Imaginary axis
- For PDE matrices - Krylov solvers/model reduction?
- Ideas from yesterday's lectures by Strakos (scattering amplitude) and Ernst (frequency domain).
- Also: Stoll, Golub, Wathen (2007)
- Note: you choose b and c!

Outline

1. Introduction
2. Calculation of Hopf points
3. Hopf detection using bifurcation theory
4. Hopf detection using Complex Analysis
5. Hopf detection using the Cayley Transform
6. Stable and unstable periodic orbits

The Cayley Transform

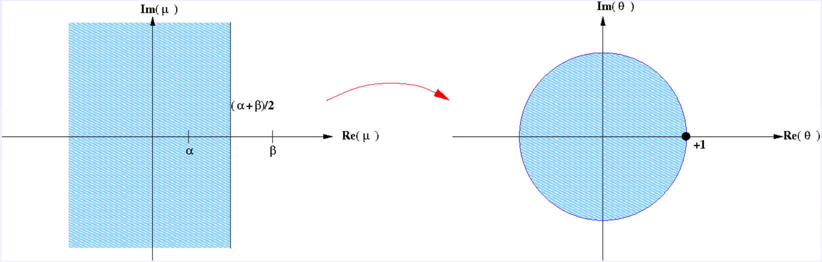


Figure: The mapping of μ to θ

- $A\phi = \mu B\phi$
- Choose α and β and form:

$$C = (A - \alpha B)^{-1}(A - \beta B) \quad \text{The Cayley transform}$$

- As λ varies, if μ crosses the line $\mathrm{Re}(\alpha+\beta)/2$ then θ moves outside the unit ball

Hopf detection using the Cayley Transform

- Mapping
$$\theta = (\mu - \alpha)^{-1}(\mu - \beta)$$
- So $\beta = -\alpha$ maps left-half plane ("stable") into unit circle
- Algorithm: At each point on $F(x, \lambda) = 0$:
  1. Choose α, β
  2. monitor dominant eigenvalues of $C = (A - \alpha B)^{-1}(A - \beta B)$
- Don't need to know $\mathrm{Im}(\mu)$
- Successfully computed Hopf bifurcations in Taylor problem and Double-diffusive convection
- BUT: "large" eigenvalues, μ, "cluster" at $\theta = 1$

Outline

1. Introduction
2. Calculation of Hopf points
3. Hopf detection using bifurcation theory
4. Hopf detection using Complex Analysis
5. Hopf detection using the Cayley Transform
6. Stable and unstable periodic orbits

Periodic orbits

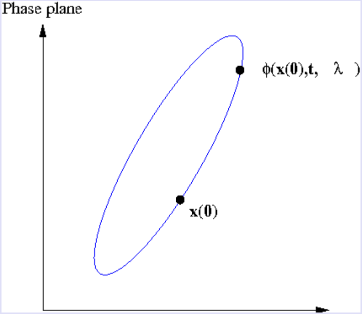
Theory

- $\dot{x} = F(x, \lambda), \quad x(t) \in \mathbb{R}^n$
- $x(0) = x(T), \quad T$=period
- Solution ("flow"): $\phi(x(0), t, \lambda)$
- Periodic: $\phi(x(0), T, \lambda) = x(0)$
- Phase condition: $s(x(0)) = 0$
- Stability: Monodromy matrix

$$\phi_x = \frac{\partial \phi}{\partial x(0)}(x(0), T, \lambda)$$

- $\mu_i \in \sigma(\phi_x)$: Floquet multipliers
- Stability: $|\mu_i| < 1, i = 2 \dots n$ $(\mu_1 = 1)$
- Monodromy matrix is FULL

Phase plane



Stability of periodic orbits

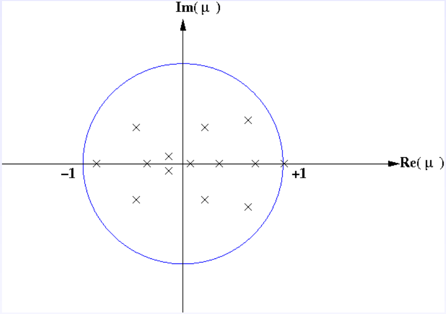


Figure: Plot of Floquet multipliers for a stable periodic orbit

- Loss of stability: multiplier crosses unit circle (e.g. real eigenvalue crosses through -1 then "period-doubling bifurcation")
- If solution is stable just integrate in time: OK if μ_i not near unit circle
- "Integrate in time" is no good for unstable orbits

Newton-Picard Method for periodic orbits (Lust et. al.)

- Unknowns: initial condition, $x(0)$, and period, T, (drop λ)
- Fixed point problem + phase condition

$$\phi(x(0), T) = x(0), \quad s(x(0)) = 0$$

Newton-Picard Method for periodic orbits (Lust et. al.)

- Unknowns: initial condition, $x(0)$, and period, T, (drop λ)
- Fixed point problem + phase condition

$$\phi(x(0), T) = x(0), \quad s(x(0)) = 0$$

- Picard Iteration: Guess $(x^{(0)}(0), T^{(0)})$ and compute $x^{(1)}(0)$

$$\phi(x^{(0)}(0), T^{(0)}) = x^{(1)}(0)$$

Newton-Picard Method for periodic orbits (Lust et. al.)

- Unknowns: initial condition, $x(0)$, and period, T, (drop λ)
- Fixed point problem + phase condition

$$\phi(x(0), T) = x(0), \quad s(x(0)) = 0$$

- Picard Iteration: Guess $(x^{(0)}(0), T^{(0)})$ and compute $x^{(1)}(0)$

$$\phi(x^{(0)}(0), T^{(0)}) = x^{(1)}(0)$$

- Newton's Method: Guess $(x(0)^{(0)}, T^{(0)})$ and compute corrections

$$\begin{bmatrix} \phi_x - I & \phi_T \\ s_x & 0 \end{bmatrix} \begin{bmatrix} \Delta x(0) \\ \Delta T \end{bmatrix} = - \begin{bmatrix} r_1 \\ r_2 \end{bmatrix}$$

Newton-Picard Method for periodic orbits (Lust et. al.)

- Unknowns: initial condition, $x(0)$, and period, T, (drop λ)
- Fixed point problem + phase condition

$$\phi(x(0), T) = x(0), \quad s(x(0)) = 0$$

- Picard Iteration: Guess $(x^{(0)}(0), T^{(0)})$ and compute $x^{(1)}(0)$

$$\phi(x^{(0)}(0), T^{(0)}) = x^{(1)}(0)$$

- Newton's Method: Guess $(x(0)^{(0)}, T^{(0)})$ and compute corrections

$$\begin{bmatrix} \phi_x - I & \phi_T \\ s_x & 0 \end{bmatrix} \begin{bmatrix} \Delta x(0) \\ \Delta T \end{bmatrix} = - \begin{bmatrix} r_1 \\ r_2 \end{bmatrix}$$

- Newton-Picard Method: Split $\mathbb{R}^n$ into “stable” and “unstable” subspaces. Convergence? - Modified Newton
  1. Picard on “stable” subspace (large)
  2. Newton on “unstable” subspace (small)
  3. Schroff&Keller: “Recursive Projection Method” - computing stable and unstable steady states using initial value codes

Newton-Picard Method for periodic orbits

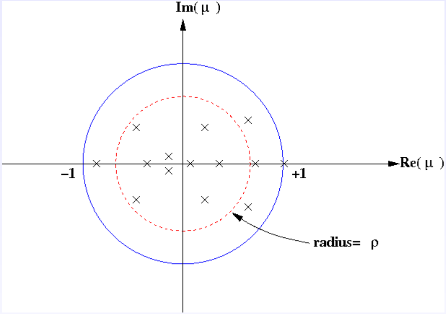
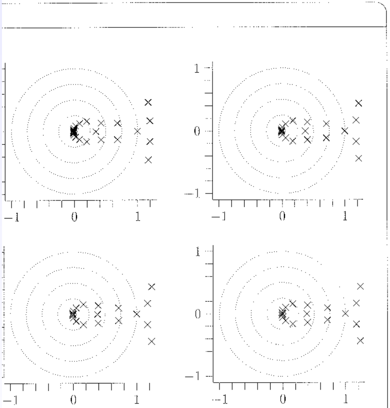


Figure: Splitting of Floquet multipliers into "stable" and "unstable" subsets

- Pick $\rho < 1$
- "Stable": $|\mu_i| < \rho$ (hopefully dimension $\approx n$)
- "Unstable":$|\mu_i| \geq \rho$ (hopefully dimension very small)

Floquet multipliers for the Brusselator

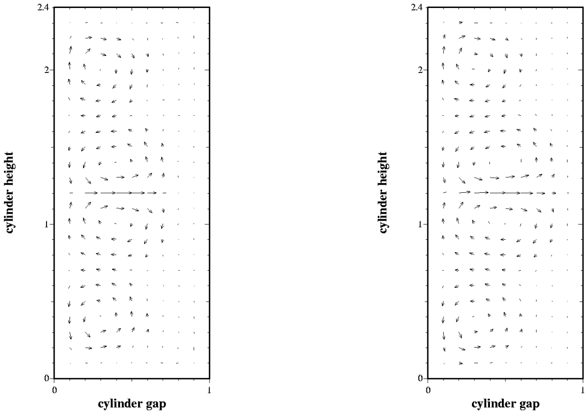


m of the Brusselator model, solution on branch VI at $L = 1.9$, with
er left), 31 (upper right), 63 (lower left) and 127 (lower right)
sation points.

Lots of Numerical Linear Algebra!

1. Find (orthogonal) basis for "unstable" space, called V
2. Construct projectors onto "unstable" and "stable" spaces
3. need the action of ϕ_x on V (implemented by a small number of ODE solves)
4. need to increase /decrease dimension of V as Floquet multipliers enter or leave the "unstable" space
5. need to compute paths of periodic orbits: use pseudo-arclength (bordered matrices)

Taylor problem with counter-rotating cylinders: Grande/Tavener/Thomas (2008)



Conclusions

- An efficient method to roughly "detect" a Hopf bifurcation in large systems is still an open problem
- Methods exist for accurate calculation once good starting values are known
- Look again at the winding number algorithm?
- Computation of stable and unstable periodic solutions for discretised PDEs (e.g. Navier-Stokes) is wide open!
- Software:
  1. LOCA "Library of Continuation Algorithms" Sandia (PDEs)
  2. MATCONT "Continuation software in Matlab": W Govaerts
  3. AUTO