

Hijacking (black-box) simulation
codes

to

compute unstable solutions

and

bifurcation behavior

Parametrized dynamical systems

Consider the parameter-dependent nonlinear dynamical system

$$\frac{d\mathbf{u}}{dt} = \mathbf{f}(\mathbf{u}, \lambda), \quad \mathbf{u} \in \mathbb{R}^N, \quad \mathbf{f} : \mathbb{R}^N \times \mathbb{R} \rightarrow \mathbb{R}^N \quad (1)$$

Some of the more interesting properties of such dynamical systems are their stable and unstable equilibrium solutions, stable and unstable periodic orbits and how these solutions vary as the parameter λ is varied.

- An *equilibrium* or *steady* solution of (1) is a solution $(\mathbf{u}^*, \lambda)$ at which $\mathbf{f}(\mathbf{u}^*, \lambda) = \mathbf{0}$
- An equilibrium solution $(\mathbf{u}^*, \lambda)$ is *stable* if for every (small) $\epsilon > 0$ there is a $\delta > 0$ such that $\|\mathbf{u}(t) - \mathbf{u}^*\| < \epsilon$ for all $t \geq 0$ and for all solutions $\mathbf{u}(t)$ of (1) satisfying $\|\mathbf{u}(0) - \mathbf{u}^*\| < \delta$
- An equilibrium solution $(\mathbf{u}_0, \lambda)$ is *asymptotically stable* if it is stable and, in addition, there exists an $r > 0$ such that $\|\mathbf{u}(t) - \mathbf{u}^*\| \rightarrow 0$ as $t \rightarrow \infty$ for all solutions $\|\mathbf{u}(0) - \mathbf{u}^*\| < r$
- If all the eigenvalues of the Jacobian matrix $\mathbf{f}_{\mathbf{u}}(\mathbf{u}^*, \lambda)$ have negative real parts, then the equilibrium solution $(\mathbf{u}^*, \lambda)$ of (1) is asymptotically stable

Numerical bifurcation techniques

- Determine properties of the *steady* solution set, i.e. $(\mathbf{u}, \lambda)$ such that $\mathbf{f}(\mathbf{u}, \lambda) = \mathbf{0}$
- Utilize results from singularity theory (see e.g. Golubitsky, Stewart & Schaeffer)
- Make appropriate use of symmetry
- Basic strategy: Solve steady (equilibrium) equations augmented by extra conditions which define the type of singularity
- Major theoretical developments
 - 1977–1987: Keller, Jepson, Spence, Werner
 - 1980–1981: Brezzi, Rappaz & Raviart
 - 1985–1990: Dellnitz, Healey
 - 1995–2000: Govaerts
- Implementation and Applications
 - 1980–1990: Cliffe & Winters
 - 1990–2000: Dijkstra, Khibnik, Nandakumar, Tuckerman
 - Software: Auto, Content, Entwife, HomCont, Matcont, Loca

Advantages

1. Efficiency cf. simulation, especially near critical points
2. Efficiency cf. simulation for multi-dimensional parameter spaces
 - (a) Locate organizing centers
 - (b) Loci of codimension-one singularities partition parameter space into regions in which qualitatively similar bifurcation behaviour occurs
3. Superconvergence property at critical points when a Galerkin method is employed. (Related to superconvergence of eigenvalue problems, see e.g. Babuska and Osborn.)
4. Independent of discretization technique

It should not matter how the system of nonlinear algebraic equations $\mathbf{f}(\mathbf{x}, \lambda) = \mathbf{0}$ is obtained, e.g. via finite element, finite difference or spectral methods.

Limitations

1. Detect *onset* of time-dependence only, e.g. at Hopf bifurcation points
2. Require evaluation of derivatives of $\mathbf{f}(\mathbf{x}, \lambda)$ with respect to both $\mathbf{x}$ and λ
3. Require solving augmented systems of equations ($3N + 2$ in the case of Hopf bifurcation points), and solving systems for multiple right-hand-sides
4. Extended system for locating Hopf bifurcation points requires a good initial guess.
(One must be able to determine when a pair of complex conjugate eigenvalues of a large, sparse, generalized eigenvalue problem cross the imaginary axis.)

Traditional applications

1. Taylor-Couette flow
2. Flow in an expanding and contracting channel
3. Flow past a rotating cylinder
4. Marangoni-Bénard convection
5. Dean flow

More exotic applications

Using computer algebra to write subroutines to evaluate derivatives etc. allows the technique to be applied to free surface flows, problems with mixed physics and complex physics, and (limited) multi-scale phenomena.

1. Free surface flow down an inclined plane with topography
2. Two-fluid Marangoni-Benard convection with a deformable interface
3. Electrohydrodynamic convection in a nematic liquid crystal
4. Multi-scale phenomena: density induced convection in a BZ mixture

Most scientific codes solve time-dependent problems

Despite ...

- Time-dependent codes fail to converge to unstable equilibria
- Time-dependent codes converge extremely slowly near bifurcation (interesting) points.

Question: Can we take advantage of the time and expertise that has been used to develop time-dependent codes in order to answer questions about the bifurcation structure of the steady solution set?

Equilibria as fixed points

Integrate the o.d.e.

$$\frac{d\mathbf{u}}{dt} = \mathbf{f}(\mathbf{u}, \lambda), \quad \mathbf{u} \in \mathbb{R}^N, \quad \mathbf{f} : \mathbb{R}^N \times \mathbb{R} \rightarrow \mathbb{R}^N$$

forward in time and look for an equilibrium.

This proceeds as: Given $\mathbf{u}(t)$,

“black-box” integrator $\longrightarrow \mathbf{u}(t + \Delta t)$,

or, equivalently: Given $\mathbf{u}^{(k)}$

“black-box” integrator $\longrightarrow \mathbf{u}^{(k+1)}$.

Thus we can consider the integrator as applying the map

$$\mathbf{u}^{(k+1)} = \mathbf{F} \left(\mathbf{u}^{(k)}; \lambda \right),$$

and observe that finding an equilibrium solution is equivalent to finding a fixed point of this map.

Fixed point iteration

Consider the iteration

$$\mathbf{u}^{(k+1)} = \mathbf{F}(\mathbf{u}^{(k)}, \lambda), \quad \mathbf{F} : \mathbb{R}^N \times \mathbb{R} \rightarrow \mathbb{R}^N \quad (2)$$

- The sequence $\{\mathbf{u}^{(k)}\}$ defined by

$$\mathbf{u}^{(k+1)} = \mathbf{F}(\mathbf{u}^{(k)}, \lambda), \quad k = 0, 1, \dots$$

converges to $\mathbf{u}^*$, iff the spectral radius $\rho(\mathbf{F}\mathbf{u}(\mathbf{u}^*)) < 1$, provided that $\mathbf{u}^{(0)}$ is sufficiently close to $\mathbf{u}^*$.

- Moreover for every $\epsilon > 0$ there is a constant C , depending only on $\mathbf{u}^{(0)}$ and ϵ but not on k , such that

$$\|\mathbf{u}^{(k)} - \mathbf{u}^*\| \leq C(\rho(\mathbf{F}\mathbf{u}(\mathbf{u}^*)) + \epsilon)^k.$$

Explicit Euler

Solving

$$\frac{d\mathbf{u}}{dt} = \mathbf{f}(\mathbf{u}, \lambda), \quad \mathbf{u} \in \mathbb{R}^N, \quad \mathbf{f} : \mathbb{R}^N \times \mathbb{R} \rightarrow \mathbb{R}^N$$

using Explicit Euler we have

$$\mathbf{u}^{(k+1)} = \mathbf{u}^{(k)} + \Delta t \mathbf{f}(\mathbf{u}^{(k)}, \lambda) \equiv \mathbf{F}(\mathbf{u}^{(k)}, \lambda) \quad (3)$$

and hence

$$\mathbf{F}\mathbf{u} = \mathbf{I} + \Delta t \mathbf{f}\mathbf{u}.$$

If $\{\mu_j\}$ and $\{\alpha_j\}, j = 1, \dots, N$ are the eigenvalues of $\mathbf{F}\mathbf{u}$ and $\mathbf{f}\mathbf{u}$ respectively, then

$$\mu_j = 1 + \Delta t \alpha_j.$$

Hence, iteration (3) is convergent if and only if

$$\mathcal{R}e(\alpha_j) < -\frac{\Delta t}{2} |\alpha_j|^2, \quad j = 1, \dots, N$$

Further, if iteration (3) is convergent with fixed point $\mathbf{u}^*$, then the equilibrium solution $\mathbf{u}^*$ of (1) is stable.

Potential problem - clustering of eigenvalues near 1 when Δt is small.

Implicit Euler

Solving

$$\frac{d\mathbf{u}}{dt} = \mathbf{f}(\mathbf{u}, \lambda), \quad \mathbf{u} \in \mathbb{R}^N, \quad \mathbf{f} : \mathbb{R}^N \times \mathbb{R} \rightarrow \mathbb{R}^N$$

using Implicit Euler we have

$$\mathbf{u}^{(k+1)} = \mathbf{u}^{(k)} + \Delta t \mathbf{f}(\mathbf{u}^{(k+1)}, \lambda) \quad (4)$$

or

$$\mathbf{u}^{(k+1)} = (I - \Delta t \mathbf{f})^{-1} \mathbf{u}^{(k)} \equiv \mathbf{F}(\mathbf{u}^{(k)}) \quad (5)$$

and hence

$$\mathbf{F}\mathbf{u} = (I - \Delta t \mathbf{f}\mathbf{u})^{-1}.$$

If $\{\mu_j\}$ and $\{\alpha_j\}, j = 1, \dots, N$ are the eigenvalues of $\mathbf{F}\mathbf{u}$ and $\mathbf{f}\mathbf{u}$ respectively, then

$$\mu_j = \frac{1}{1 - \Delta t \alpha_j}.$$

Potential problem - clustering of eigenvalues near 1 when Δt is small.

The dynamics of a rod and spring system under a vertical load

The potential energy of the rigid rod and linear torsional spring system is

$$V = Pl \cos \alpha + \frac{1}{2}k\alpha^2.$$

For equilibrium, we require that

$$\begin{aligned} \frac{\partial V}{\partial \alpha} &= -Pl \sin \alpha + k\alpha = 0, \\ \text{i.e. } f(\alpha, \lambda) &= \alpha - \lambda \sin \alpha = 0, \text{ where } \lambda = \frac{Pl}{k} > 0. \end{aligned}$$

Equilibrium behavior

- $\alpha = 0$ for all $\lambda > 0$
- $\alpha / \sin \alpha = \lambda$ for all $\lambda > 1$
- If α is a solution, then so is $-\alpha$
- $\lim_{\lambda \rightarrow \infty} \alpha = 0, \pm\pi$

There is a symmetry-breaking supercritical pitchfork bifurcation at $\lambda = 1$.

Dynamics

$$\frac{\partial^2 \alpha}{dt^2} = -\alpha + \lambda \sin \alpha$$

or

$$\begin{pmatrix} \dot{\alpha}_1 \\ \dot{\alpha}_2 \end{pmatrix} = \mathbf{f}(\boldsymbol{\alpha}; \lambda) = \begin{pmatrix} \alpha_2 \\ -\alpha_1 + \lambda \sin \alpha_1 \end{pmatrix} .$$

Adding some velocity damping

$$\frac{\partial^2 \alpha}{dt^2} = -\alpha + \lambda \sin \alpha - \omega \frac{\partial \alpha}{dt} ,$$

or

$$\begin{pmatrix} \dot{\alpha}_1 \\ \dot{\alpha}_2 \end{pmatrix} = \mathbf{f}(\boldsymbol{\alpha}; \lambda) = \begin{pmatrix} \alpha_2 \\ -\alpha_1 + \lambda \sin \alpha_1 - \omega \alpha_2 \end{pmatrix} .$$

(a) *Explicit Euler*

Solve

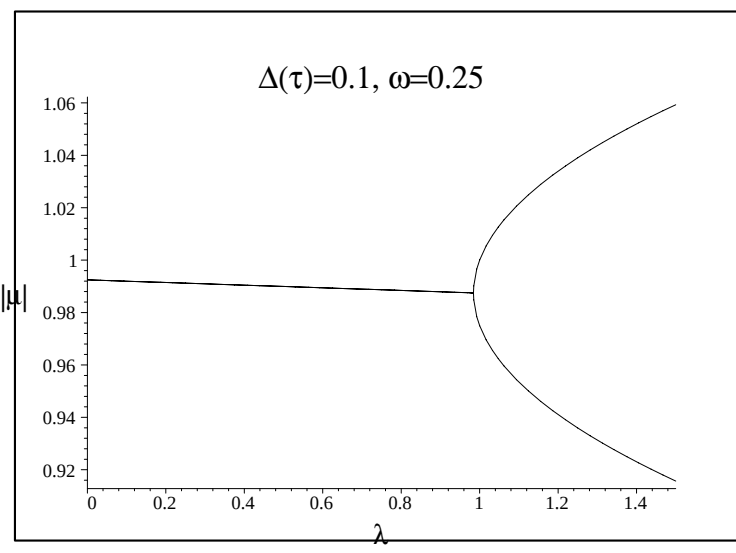
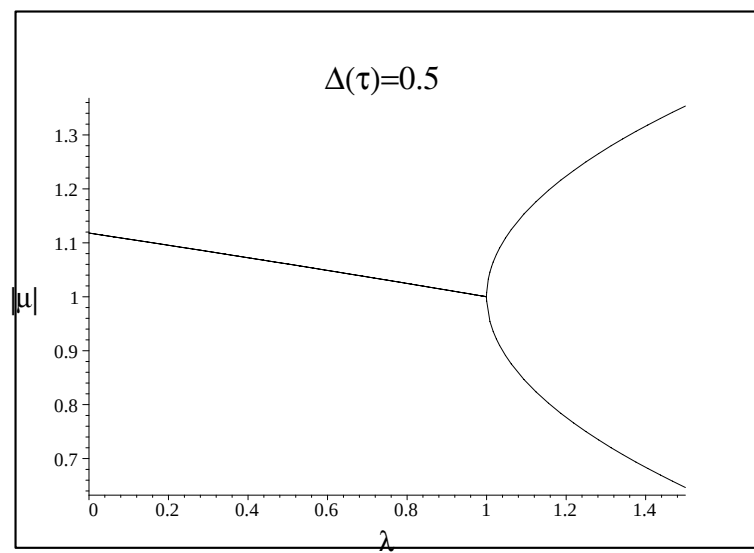
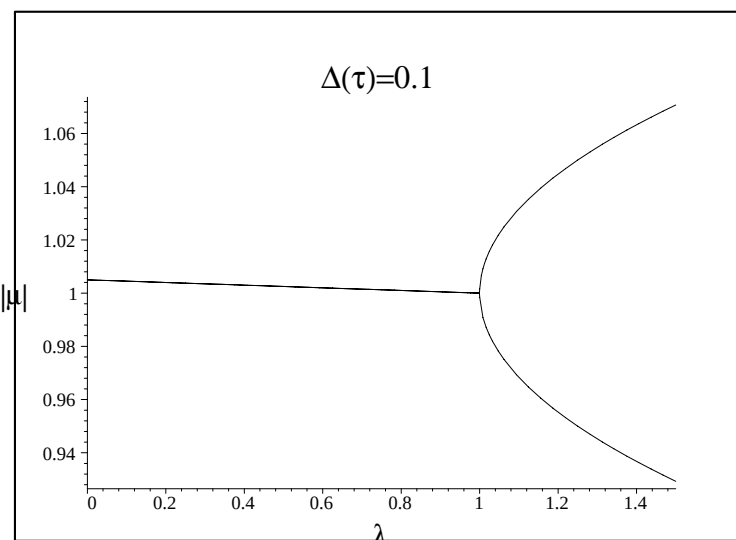
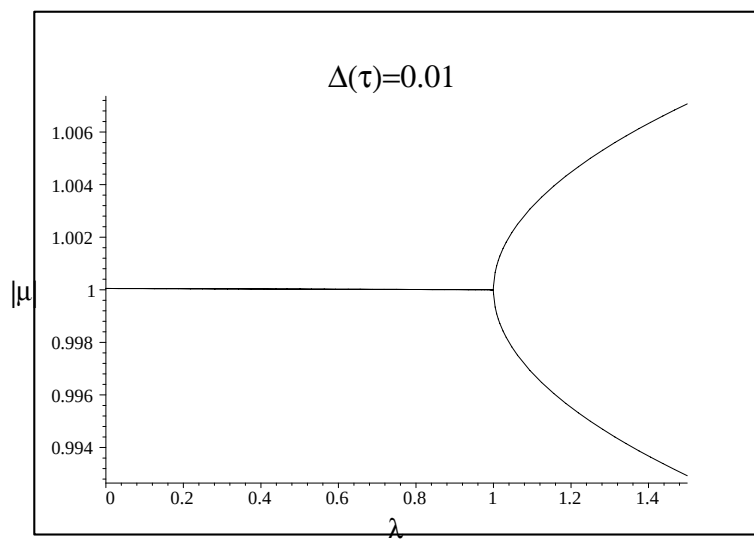
$$\begin{aligned}\boldsymbol{\alpha}^{(k+1)} &= \boldsymbol{\alpha}^{(k)} + \boldsymbol{f}(\boldsymbol{\alpha}^{(k)}; \lambda) \Delta t \\ &= \boldsymbol{F}(\boldsymbol{\alpha}^{(k)}).\end{aligned}$$

Thus

$$\begin{aligned}\frac{\partial \boldsymbol{F}}{\partial \boldsymbol{\alpha}} &= \boldsymbol{I} + \frac{\partial \boldsymbol{f}}{\partial \boldsymbol{\alpha}} \Delta t \\ &= \begin{bmatrix} 1 & \Delta t \\ (\lambda \cos(\alpha_1) - 1) \Delta t & 1 - \omega \Delta t \end{bmatrix}\end{aligned}$$

for our example problem.

– See Maple for spectrum as a function of λ , for $\alpha_1 = 0$.



(b) *Implicit Euler*

Solve

$$\boldsymbol{\alpha}^{(k+1)} - \boldsymbol{f}(\boldsymbol{\alpha}^{(k+1)}; \lambda) \Delta t - \boldsymbol{\alpha}^{(k)} = \mathbf{0}.$$

This can be recast as a fixed point iteration

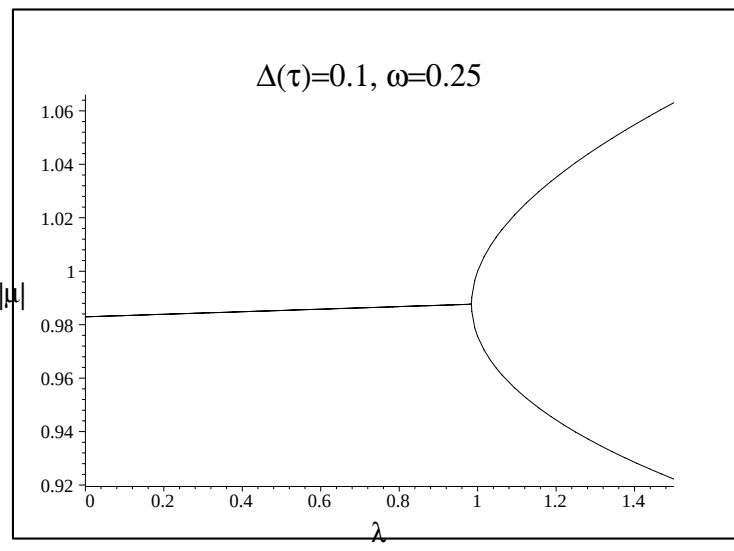
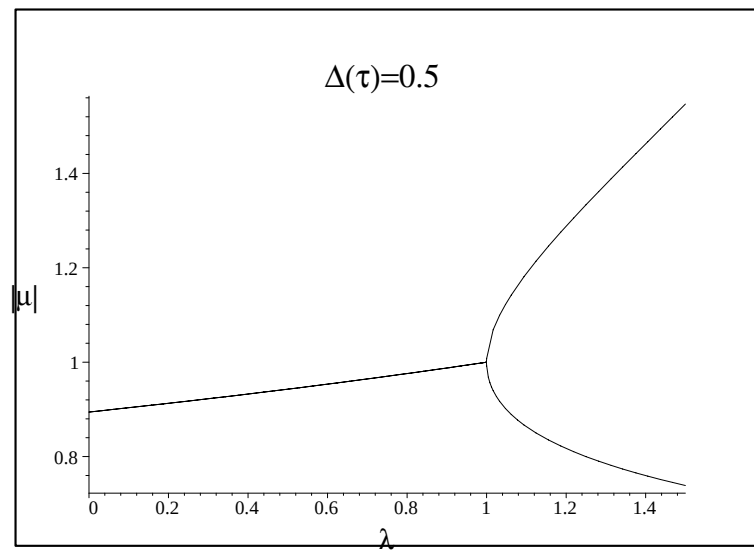
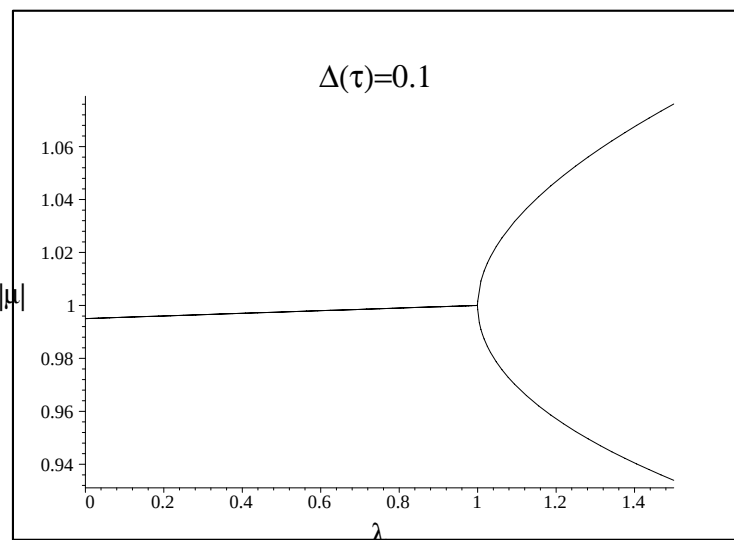
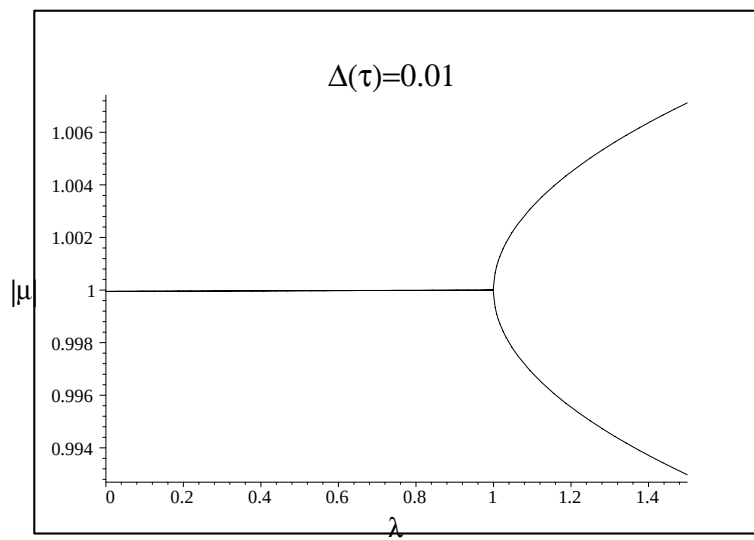
$$\boldsymbol{\alpha}^{(k+1)} = \boldsymbol{G}(\boldsymbol{\alpha}^{(k)})$$

with Jacobian

$$\begin{aligned} \frac{\partial \boldsymbol{G}}{\partial \boldsymbol{\alpha}} &= \left(\boldsymbol{I} - \frac{\partial \boldsymbol{f}}{\partial \boldsymbol{\alpha}} \Delta t \right)^{-1}, \\ &= \begin{bmatrix} 1 & -\Delta t \\ -(\lambda \cos(\alpha_1) - 1) \Delta t & 1 + \omega \Delta t \end{bmatrix}^{-1} \end{aligned}$$

for our example problem.

– See Maple for spectrum as a function of λ , for $\alpha_1 = 0$.



The essential splitting idea

Consider the map

$$\mathbf{u}^{(k+1)} = \mathbf{F}(\mathbf{u}^{(k)}; \lambda). \quad (6)$$

Let the Jacobian matrix $\mathbf{M}^{(k)} = \mathbf{F}_{\mathbf{u}}(\mathbf{u}^{(k)}; \lambda)$ have eigenvalues μ_i , $i = 1, \dots, N$ such that

$$|\mu_1| \geq \dots \geq |\mu_p| > 1 - \delta > |\mu_{p+1}| \geq \dots \geq |\mu_N|$$

Let $\mathcal{P}$ be the p -dimensional subspace spanned by the eigenvectors and generalized eigenvectors of $\mathbf{M}^{(k)}$ corresponding to $\mu_1, \dots, \mu_p$. Let $\mathcal{Q} = \mathcal{P}^\perp$. Let $\mathbf{V}_P$ be an orthonormal basis for $\mathcal{P}$ and let

$$\begin{aligned} \mathbf{P} &= \mathbf{V}_P \mathbf{V}_P^T, \\ \mathbf{Q} &= \mathbf{V}_Q \mathbf{V}_Q^T = \mathbf{I} - \mathbf{P}, \end{aligned}$$

be orthogonal projectors onto $\mathcal{P}$ and $\mathcal{Q}$ respectively. For any $\mathbf{u} \in \mathbb{R}^N$,

$$\mathbf{u} = \mathbf{P}\mathbf{u} + \mathbf{Q}\mathbf{u} = \mathbf{p} + \mathbf{q}.$$

Recursive Projection Method

Split the map (6) as into the two (unequal) pieces

$$\begin{aligned}\mathbf{p}^{(k+1)} &= \mathbf{P}\mathbf{u}^{(k+1)} \\ &= \mathbf{P}\mathbf{F}(\mathbf{u}^{(k)}; \lambda) \\ &= \mathbf{P}\mathbf{F}(\mathbf{p}^{(k)} + \mathbf{q}^{(k)}; \lambda) \\ &= \mathbf{f}(\mathbf{p}^{(k)}, \mathbf{q}^{(k)}; \lambda),\end{aligned}\tag{7}$$

and

$$\begin{aligned}\mathbf{q}^{(k+1)} &= \mathbf{Q}\mathbf{u}^{(k+1)} \\ &= \mathbf{Q}\mathbf{F}(\mathbf{u}^{(k)}; \lambda) \\ &= \mathbf{Q}\mathbf{F}(\mathbf{p}^{(k)} + \mathbf{q}^{(k)}; \lambda) \\ &= \mathbf{g}(\mathbf{p}^{(k)}, \mathbf{q}^{(k)}; \lambda).\end{aligned}\tag{8}$$

Note that the spectral radius of

$$r_\sigma(\mathbf{g}_q) = r_\sigma(\mathbf{Q}\mathbf{F}_u\mathbf{Q}) \leq 1 - \delta < 1.$$

Strategy:

Apply the iteration

$$\mathbf{q}^{(k+1)} = \mathbf{g}(\mathbf{p}^{(k)}, \mathbf{q}^{(k)}; \lambda) \text{ (equation 8), to compute } \mathbf{q}^{(k+1)}$$

and then find

$$\mathbf{p}^{(k+1)} \text{ from } \mathbf{p}^{(k+1)} = \mathbf{f}(\mathbf{p}^{(k)}, \mathbf{q}^{(k)}; \lambda) \text{ (equation 7), by Newton's method,}$$

i.e., solve $\mathbf{p} - \mathbf{f}(\mathbf{p} + \mathbf{q}; \lambda) = \mathbf{0}$ by the following Newton iteration

$$\begin{aligned} [\mathbf{I} - \mathbf{f}_p^{(k)}] \Delta \mathbf{p}^{(k)} &= -\mathbf{p}^{(k)} + \mathbf{f}^{(k)}, \\ \mathbf{p}^{(k+1)} &= \mathbf{p}^{(k)} + \Delta \mathbf{p}^{(k)} \end{aligned}$$

where

$$\mathbf{f}_p = \mathbf{P} \mathbf{F}_u \mathbf{P}.$$

Note that RPM is a Jacobi like iteration, since $\mathbf{q}^{(k+1)}$ is not used to compute $\mathbf{p}^{(k+1)}$.

Convergence: RPM (Shroff & Keller, 1993)

Note that

1. $\mathbf{QF_uP} = \mathbf{0}$ since $\mathcal{P}$ is an invariant subspace,
2. $r_\sigma(\mathbf{g}_q) = r_\sigma(\mathbf{QF_uQ}) \leq 1 - \delta < 1$.

We can represent the RPM iteration as the fixed point iteration

$$\begin{aligned}\mathbf{p}^{(k+1)} &= \mathbf{h}(\mathbf{p}^{(k)}, \mathbf{q}^{(k)}; \lambda), \\ \mathbf{q}^{(k+1)} &= \mathbf{g}(\mathbf{p}^{(k)}, \mathbf{q}^{(k)}; \lambda),\end{aligned}$$

where

$$\mathbf{h}(\mathbf{p}, \mathbf{q}, \lambda) = \mathbf{p} + (\mathbf{I} - \mathbf{f}_p)^{-1}(\mathbf{f} - \mathbf{p}).$$

At the fixed point $\mathbf{u}^*$, the Jacobian

$$\begin{aligned}\frac{\partial(\mathbf{h}, \mathbf{g})}{\partial(\mathbf{p}, \mathbf{q})} &= \begin{bmatrix} \mathbf{I} + (\mathbf{I} - \mathbf{f}_p)^{-1}(\mathbf{f}_p - \mathbf{I}) & (\mathbf{I} - \mathbf{f}_p)^{-1}\mathbf{f}_q \\ \mathbf{g}_p & \mathbf{g}_q \end{bmatrix} \\ &= \begin{bmatrix} \mathbf{0} & (\mathbf{I} - \mathbf{f}_p)^{-1}\mathbf{f}_q \\ \mathbf{0} & \mathbf{g}_q \end{bmatrix}\end{aligned}$$

and thus has spectral radius $\leq 1 - \delta < 1$.

Newton-Picard iteration

Solve $\mathbf{F}(\mathbf{u}; \lambda) - \mathbf{u} = \mathbf{0}$ by Newton iteration, i.e. at each iteration solve

$$[\mathbf{M}^{(k)} - \mathbf{I}] \Delta \mathbf{u}^{(k)} = -\mathbf{r}^{(k)}, \quad (9)$$

where $\mathbf{r}^{(k)} = \mathbf{F}(\mathbf{u}^{(k)}; \lambda) - \mathbf{u}^{(k)}$.

We split the Newton iteration (9) to yield

$$\begin{aligned} \mathbf{V}_P^T [\mathbf{M}^{(k)} - \mathbf{I}] \Delta \mathbf{u}^{(k)} &= -\mathbf{V}_P^T \mathbf{r}^{(k)}, \\ \mathbf{V}_Q^T [\mathbf{M}^{(k)} - \mathbf{I}] \Delta \mathbf{u}^{(k)} &= -\mathbf{V}_Q^T \mathbf{r}^{(k)}, \end{aligned}$$

and for convenience we define local coordinates in $\mathcal{P}$ and $\mathcal{Q}$,

$$\begin{aligned} \bar{\mathbf{p}} &= \mathbf{V}_P^T \mathbf{u} \in \mathbb{R}^p, \\ \bar{\mathbf{q}} &= \mathbf{V}_Q^T \mathbf{u} \in \mathbb{R}^q. \end{aligned}$$

Splitting the Newton iteration (9) yields

$$\begin{aligned}
\mathbf{V}_P^T [\mathbf{M}^{(k)} - \mathbf{I}] \Delta \mathbf{u}^{(k)} &= -\mathbf{V}_P^T \mathbf{r}^{(k)} \\
\mathbf{V}_P^T [\mathbf{M}^{(k)} - \mathbf{I}] \left(\mathbf{V}_P \Delta \bar{\mathbf{p}}^{(k)} + \mathbf{V}_Q \Delta \bar{\mathbf{q}}^{(k)} \right) &= -\mathbf{V}_P^T \mathbf{r}^{(k)} \\
\mathbf{V}_P^T [\mathbf{M}^{(k)} - \mathbf{I}] \mathbf{V}_P \Delta \bar{\mathbf{p}}^{(k)} + \mathbf{V}_P^T \mathbf{M}^{(k)} \mathbf{V}_Q \Delta \bar{\mathbf{q}}^{(k)} &= -\mathbf{V}_P^T \mathbf{r}^{(k)},
\end{aligned} \tag{10}$$

and

$$\begin{aligned}
\mathbf{V}_Q^T [\mathbf{M}^{(k)} - \mathbf{I}] \Delta \mathbf{u}^{(k)} &= -\mathbf{V}_Q^T \mathbf{r}^{(k)} \\
\mathbf{V}_Q^T [\mathbf{M}^{(k)} - \mathbf{I}] \left(\mathbf{V}_P \Delta \bar{\mathbf{p}}^{(k)} + \mathbf{V}_Q \Delta \bar{\mathbf{q}}^{(k)} \right) &= -\mathbf{V}_Q^T \mathbf{r}^{(k)} \\
\mathbf{V}_Q^T [\mathbf{M}^{(k)} - \mathbf{I}] \mathbf{V}_Q \Delta \bar{\mathbf{q}}^{(k)} &= -\mathbf{V}_Q^T \mathbf{r}^{(k)},
\end{aligned} \tag{11}$$

since $\mathcal{P}$ is an invariant subspace of $\mathbf{M}^{(k)}$.

Note

- (1) $[\mathbf{M}^{(k)} - \mathbf{I}]$ may be poorly conditioned.
- (2) We refer to (10) as the P -equations and (11) as the Q -equations.

Rewriting the P - and Q -equations as a block diagonal system

$$\begin{bmatrix} V_Q^T(M^{(k)} - I)V_Q & 0 \\ V_P^T M^{(k)} V_Q & V_P^T(M^{(k)} - I)V_P \end{bmatrix} \begin{pmatrix} \Delta \bar{\mathbf{q}}^{(k)} \\ \Delta \bar{\mathbf{p}}^{(k)} \end{pmatrix} = - \begin{pmatrix} V_Q^T \mathbf{r}^{(k)} \\ V_P^T \mathbf{r}^{(k)} \end{pmatrix}.$$

Since $r_\sigma(V_Q^T M^{(k)} V_Q) < 1$, the Neumann series for $[V_Q^T(\mathbf{M}^{(k)} - \mathbf{I})V_Q]^{-1}$ is convergent and we can solve the Q -equations using the power series

$$\Delta \bar{\mathbf{q}}^{(k)} \approx \sum_{k=0}^{l-1} \left(\mathbf{V}_Q^T \mathbf{M}^{(k)} \mathbf{V}_Q \right)^k \mathbf{V}_Q^T \mathbf{r}^{(k)}, \quad (12)$$

for some $l \geq 1$.

Substitute $\Delta \bar{\mathbf{q}}^{(k)}$ from (12) into the P -equations and solve

$$\mathbf{V}_P^T[\mathbf{M}^{(k)} - \mathbf{I}]\mathbf{V}_P \Delta \bar{\mathbf{p}}^{(k)} = -\mathbf{V}_P^T \mathbf{r}^{(k)} - \mathbf{V}_P^T \mathbf{M}^{(k)} \mathbf{V}_Q \Delta \bar{\mathbf{q}}^{(k)}. \quad (13)$$

Note

- (1) $\mathbf{V}_Q^T \mathbf{M}^{(k)} \mathbf{V}_Q$ may have a spectral radius close to one.
- (2) Newton-Picard is a Gauss-Seidel like iteration, since $\mathbf{q}^{(k+1)}$ is used to compute $\mathbf{p}^{(k+1)}$.

Convergence: Newton-Picard iteration (Lust et al, 1998)

We can rewrite the Newton-Picard iteration as the fixed point procedure

$$\mathbf{u}^{(k+1)} = \mathbf{u}^{(k)} + \mathbf{H}(\mathbf{u}^{(k)})\mathbf{r}(\mathbf{u}^{(k)}), \quad (14)$$

where combining (12) and (13)

$$\begin{aligned} \mathbf{H}(\mathbf{u}) = & \mathbf{V}_Q \left(\sum_{k=0}^{l-1} (\mathbf{V}_Q^T \mathbf{M}^{(k)} \mathbf{V}_Q)^k \right) \mathbf{V}_Q^T \\ & + \left(\mathbf{V}_P (\mathbf{I}_P - \mathbf{V}_P^T \mathbf{M} \mathbf{V}_P)^{-1} \mathbf{V}_P^T \right) \left(\mathbf{I} + \mathbf{M} \mathbf{V}_Q \left(\sum_{k=0}^{l-1} (\mathbf{V}_Q^T \mathbf{M}^{(k)} \mathbf{V}_Q)^k \right) \mathbf{V}_Q^T \right). \end{aligned}$$

At the fixed point $\mathbf{u}^*$ the Jacobian $\mathbf{G}$ of the fixed point iteration (14) is

$$\mathbf{G}(\mathbf{u}^*) = \mathbf{I} + \mathbf{H}(\mathbf{u}^*)\mathbf{r}_{\mathbf{u}}(\mathbf{u}^*)$$

since $\mathbf{r}(\mathbf{u}^*) = \mathbf{0}$). The spectral radius

$$r_{\sigma}[\mathbf{G}(\mathbf{u}^*)] = r_{\sigma}[\mathbf{V}^T \mathbf{G}(\mathbf{u}^*) \mathbf{V}]$$

where $\mathbf{V} = [\mathbf{V}_P | \mathbf{V}_Q]$ and

$$\mathbf{V}^T \mathbf{G}(\mathbf{u}^*) \mathbf{V} = \begin{bmatrix} (\mathbf{V}_Q^T \mathbf{M} \mathbf{V}_Q)^l & 0 \\ \star & 0 \end{bmatrix}.$$

Implementation details

Since $\mathbf{V}_Q \bar{\mathbf{q}} = \mathbf{q}$, we solve for $\Delta \mathbf{q}$ as follows

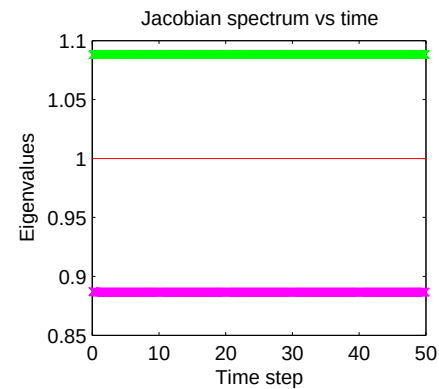
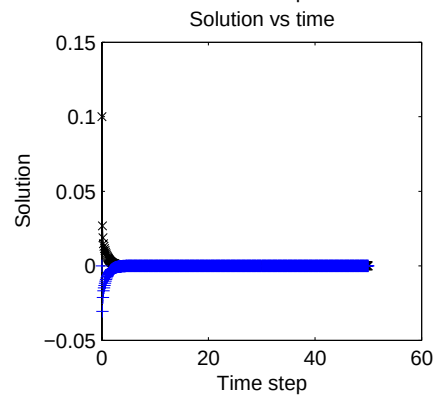
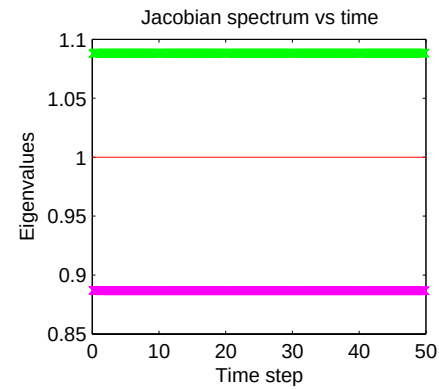
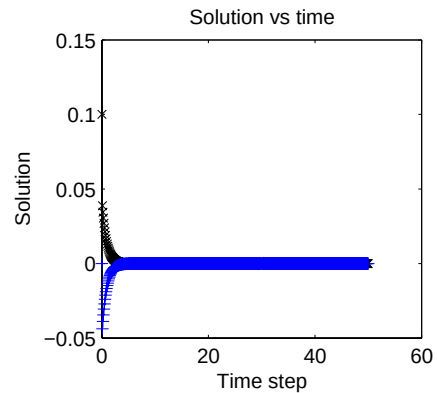
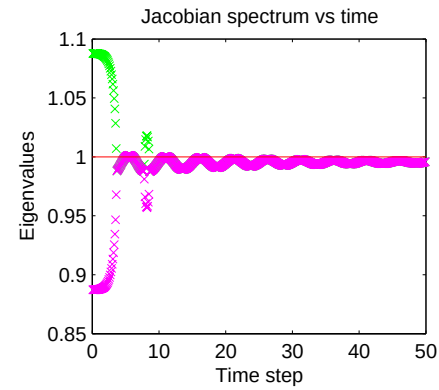
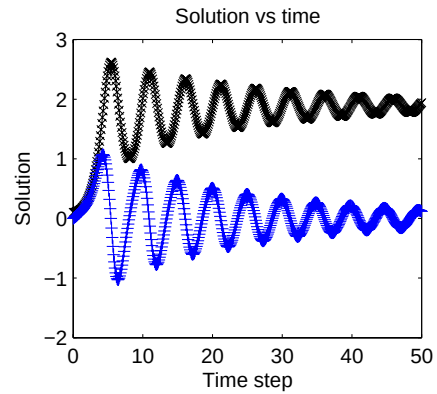
$$\begin{aligned}\Delta \mathbf{q}^{(0)} &= \mathbf{0} \\ \Delta \mathbf{q}^{(k)} &= \mathbf{Q} \mathbf{M} \Delta \mathbf{q}^{(k-1)} + \mathbf{Q} \mathbf{r}, \quad k = 1, \dots, l\end{aligned}$$

Where we note that since

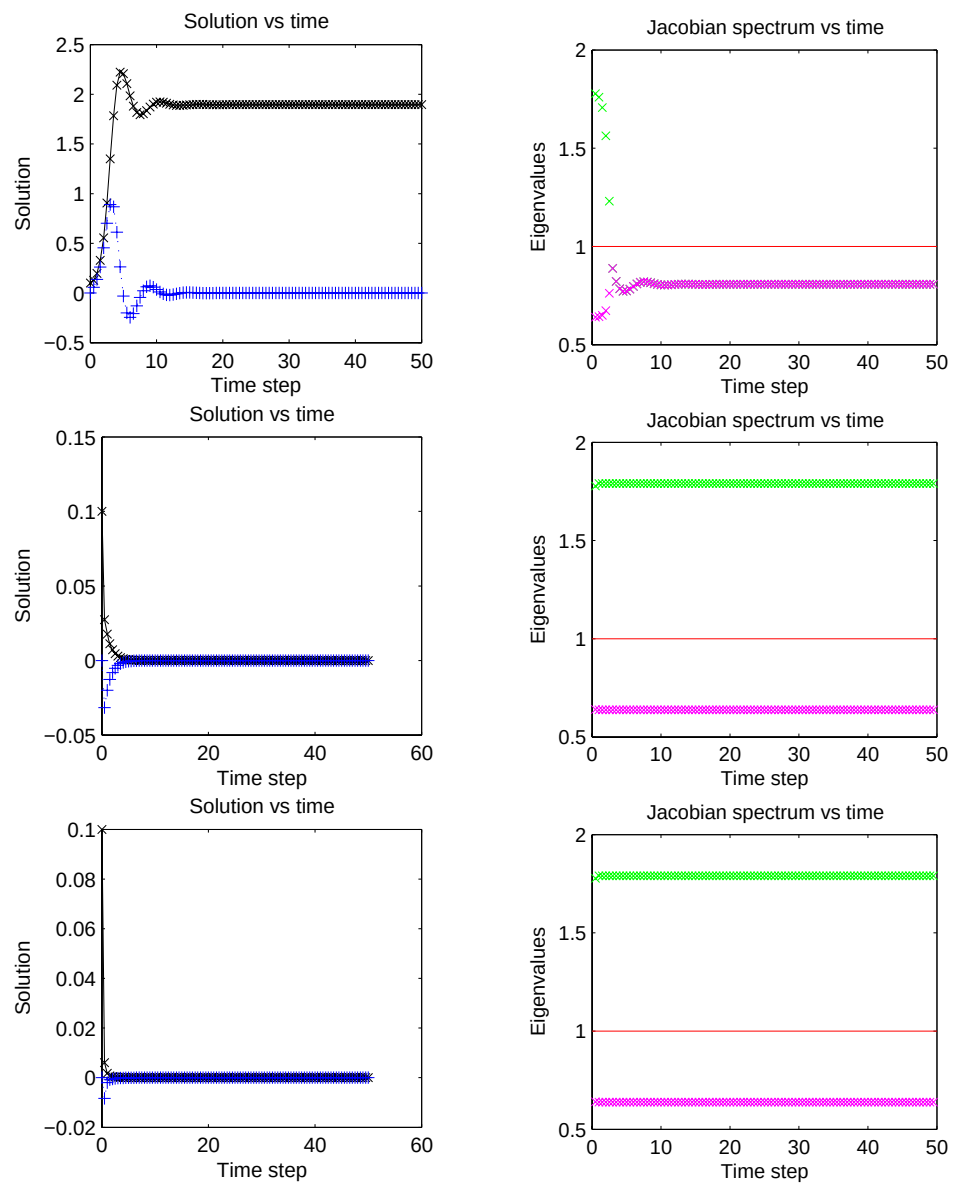
$$\mathbf{Q} = \mathbf{I} - \mathbf{P} = \mathbf{I} - \mathbf{V}_P \mathbf{V}_P^T$$

only the action of the small matrix $\mathbf{V}_P$ and its transpose is required.

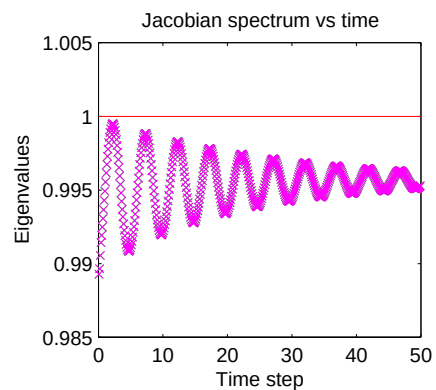
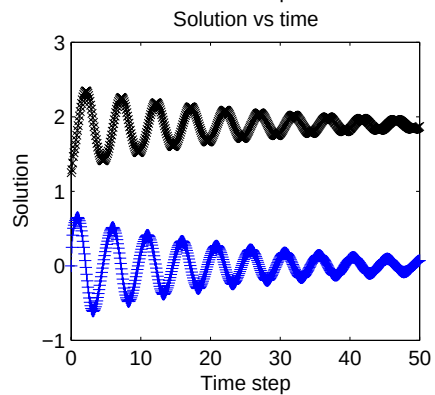
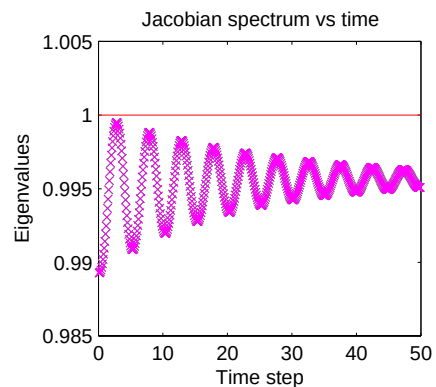
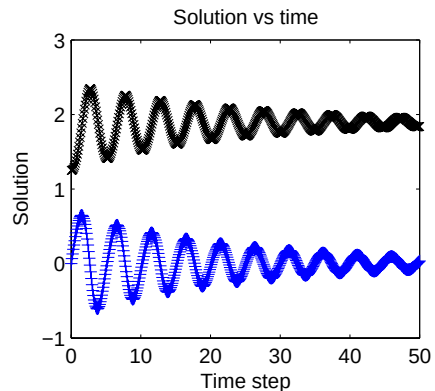
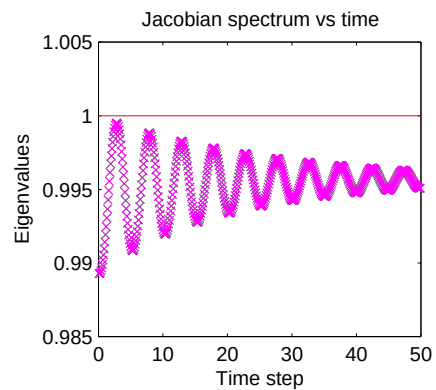
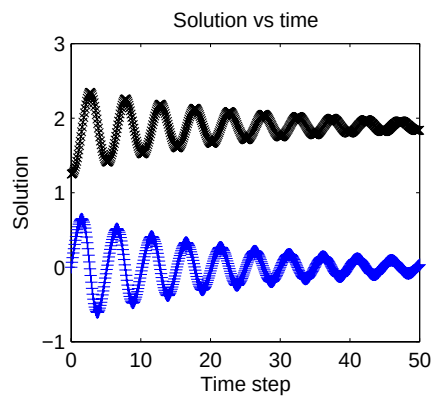
Elastic rod, Explicit Euler (Integration vs RPM vs Newton-Picard)



Elastic rod, Implicit Euler (Integration vs RPM vs Newton-Picard)



Elastic rod, Explicit Euler (Integration vs RPM vs Newton-Picard)



The dynamics of a two rod and spring system under a vertical load

The potential energy of the rigid rod and linear torsional spring system is

$$V = P(l_2 + l_1 \cos(\alpha)) \cos \beta + \frac{1}{2}k_1\alpha^2 + \frac{1}{2}k_2\beta^2.$$

For equilibrium, we require that the partial derivatives w.r.t. both α and β vanish and introducing nondimensional parameters

$$\mu = \frac{k_1}{k_2}, \quad \nu = \frac{l_1}{l_2}, \quad \lambda = \frac{Pl_2}{k_2}$$

the equilibrium equations are

$$\begin{aligned} \alpha - \lambda \frac{\nu}{\mu} \sin \alpha \cos \beta &= 0, \\ \beta - \lambda(1 + \nu \cos \alpha) \sin \beta &= 0, \end{aligned}$$

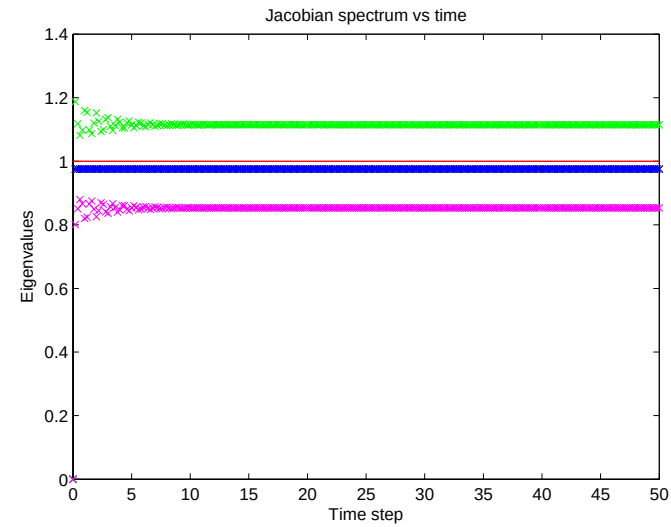
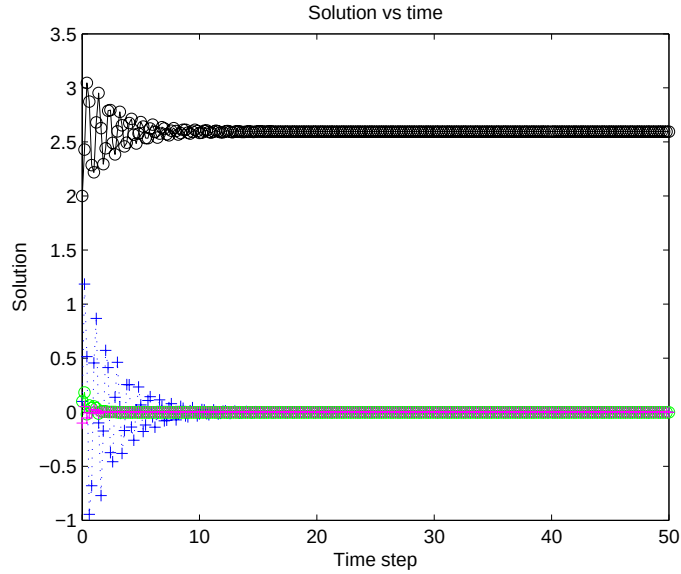
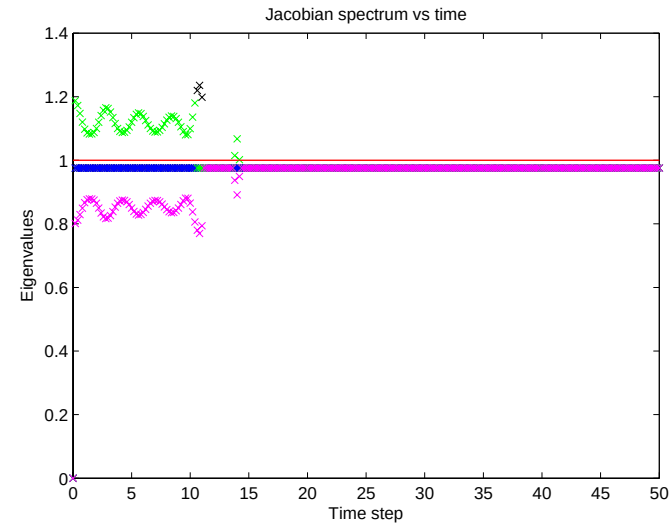
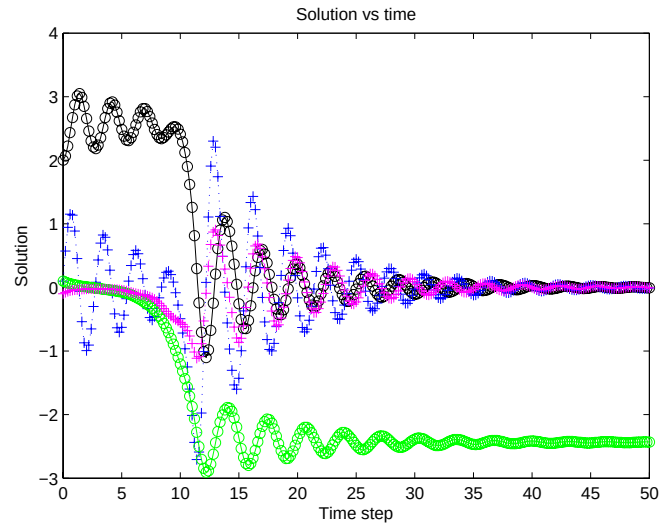
Dynamics

$$\begin{aligned} \frac{\partial^2 \alpha}{\partial t^2} &= -\alpha + \lambda \frac{\nu}{\mu} \sin \alpha \cos \beta \\ \frac{\partial^2 \beta}{\partial t^2} &= -\beta + \lambda(1 + \nu \cos \alpha) \sin \beta \end{aligned}$$

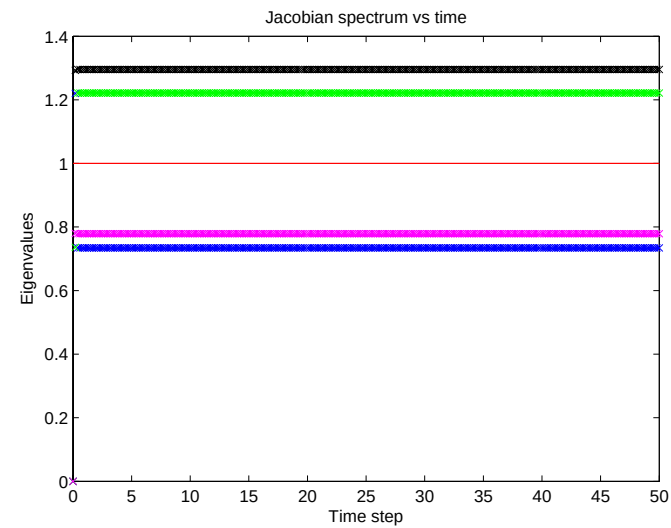
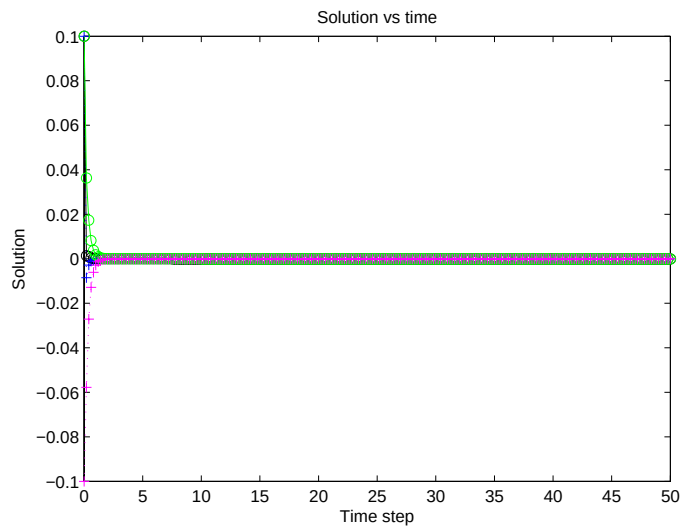
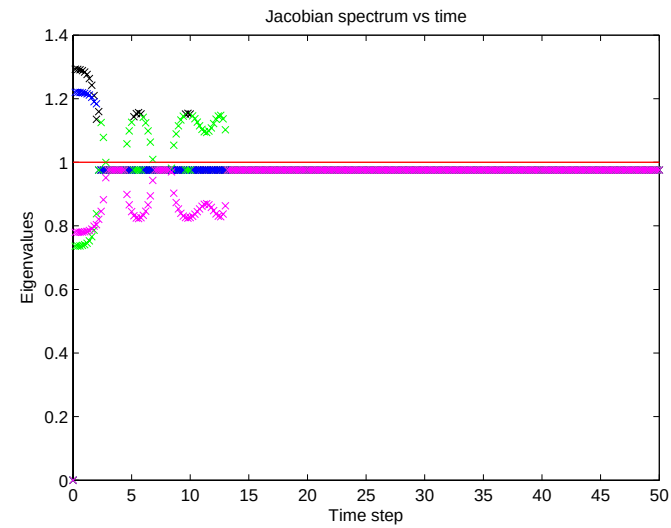
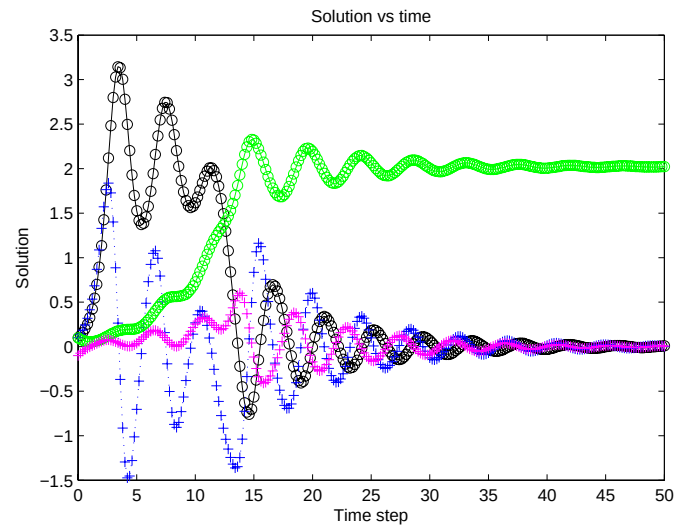
Adding some velocity damping and write as a first order system

$$\begin{pmatrix} \dot{\alpha}_1 \\ \dot{\alpha}_2 \\ \dot{\alpha}_3 \\ \dot{\alpha}_4 \end{pmatrix} = \begin{pmatrix} \alpha_2 \\ -\alpha_1 + \lambda \frac{\nu}{\mu} \sin \alpha_1 \cos \alpha_3 - \omega \alpha_2 \\ \alpha_4 \\ -\alpha_3 + \lambda(1 + \nu \cos \alpha_1) \sin \alpha_3 - \omega \alpha_4 \end{pmatrix}.$$

Two rods, $\lambda = 2.5, \mu = 1, \nu = 0.5$ (Integration vs Newton-Picard)



Two rods, $\lambda = 1.5, \mu = 1, \nu = 0.5$ (Integration vs Newton-Picard)



Taylor-Couette flow

We examine the axisymmetric flow of a Newtonian fluid contained in the annular gap between two concentric cylinders. The flow is driven by rotation of the inner and outer cylinders. The top and bottom surfaces are stationary. In our calculations,

$$\begin{aligned}\text{Aspect ratio, } \tau &= \frac{L}{d} = 2.4, \text{ where } d = r_2 - r_1 \\ \text{Radius ratio, } \eta &= \frac{r_1}{r_2} = 0.615 \\ \text{Reynolds number, } R &= \frac{\Omega_1 r_1 d}{\nu} (= 300) \\ \text{Relative velocity, } \delta &= \frac{\Omega_2 r_2}{\Omega_1 r_1}\end{aligned}$$

We used a finite difference discretization in space and the Chorin-Témam projection method in time to solve the Navier-Stokes equations

$$\begin{aligned}\frac{\partial \mathbf{u}}{\partial t} &= -\nabla p + \nabla^2 \mathbf{u} - R(\mathbf{u} \cdot \nabla \mathbf{u}), \\ 0 &= \nabla \cdot \mathbf{u}.\end{aligned}$$

The time scale $t_{scale} = d^2/\nu \approx (1\text{cm})^2/0.01\text{cm}^2\text{sec}^{-1} = 100\text{sec}$.

Chorin-Témam projection method – Chorin (1968, 1969), Temam (1969), Shen (1992, 1996)

$$\mathbf{u}^{(k+1)} = \mathbf{u}^{\text{int}} - \Delta t \nabla p^{(k+1)} \quad (15)$$

$$\nabla^2 p^{(k+1)} = \frac{1}{\Delta t} (\nabla \cdot \mathbf{u}^{\text{int}}) \quad (16)$$

where

$$\mathbf{u}^{\text{int}} = \mathbf{u}^{(k)} + \Delta t \mathbf{f}(\mathbf{u}^{(k)}) \quad (17)$$

$$\mathbf{f}(\mathbf{u}) = \nabla^2 \mathbf{u} - R(\mathbf{u} \cdot \nabla \mathbf{u}). \quad (18)$$

Evaluate $\mathbf{u}^{\text{int}}$ using (17), solve (16) for the $p^{(k+1)}$ then substitute into (15) to calculate $\mathbf{u}^{(k+1)}$.

We can rewrite this as

$$\mathbf{u}^{(k+1)} = \mathbf{u}^{\text{int}} - \Delta t \nabla \left(\nabla^{-2} \left(\frac{1}{\Delta t} \nabla \cdot \mathbf{u}^{\text{int}} \right) \right) \quad (19)$$

which indicates that the fixed point iteration is of the form

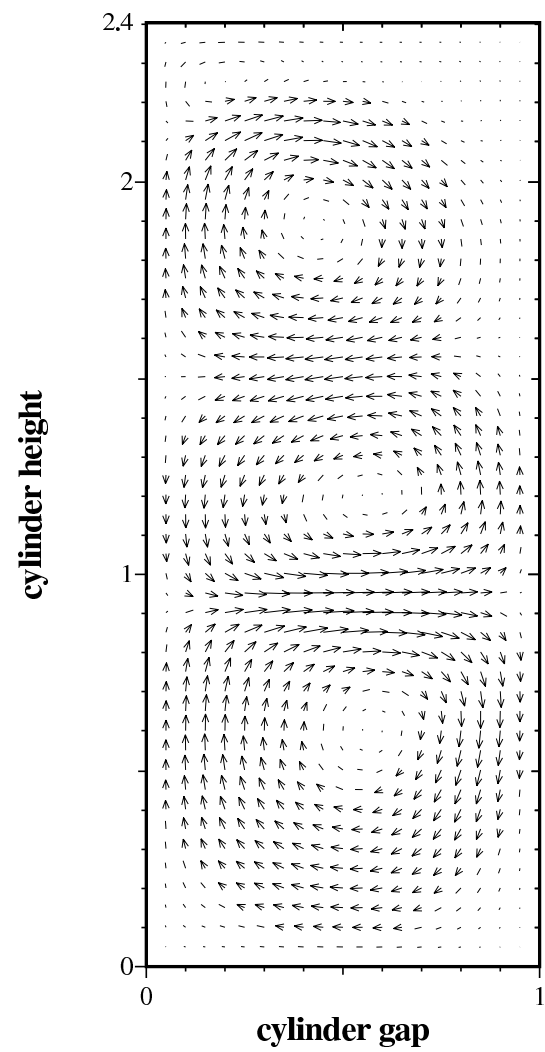
$$\mathbf{F} : \mathbf{u} \rightarrow \mathbf{u}.$$

Note: Equation (15) can be considered a projection on to a divergence-free vector field, since

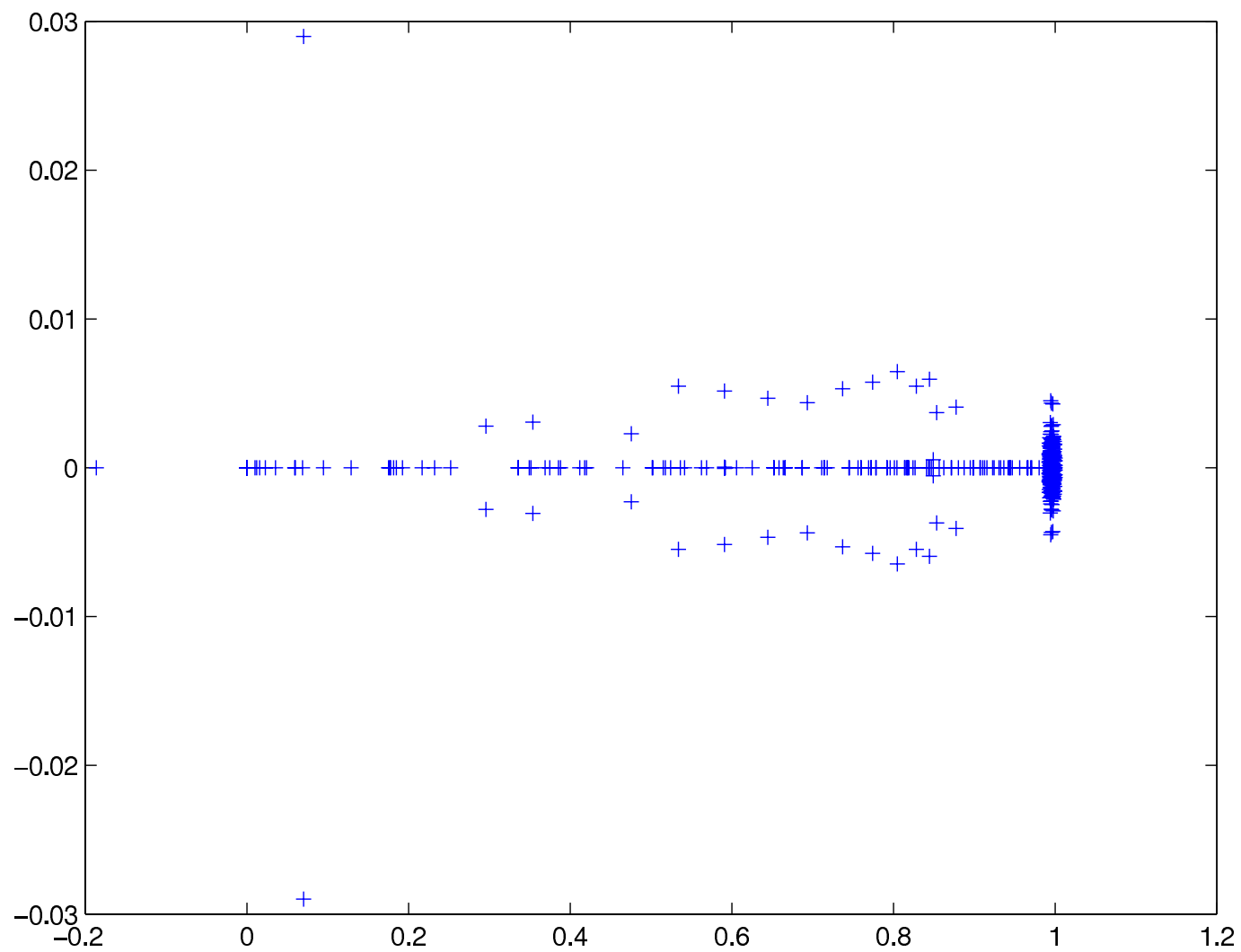
$$\begin{aligned} \nabla \cdot \mathbf{u}^{(k+1)} &= \nabla \cdot \mathbf{u}^{\text{int}} - \Delta t \nabla^2 p^{(k+1)} \\ &= \nabla \cdot \mathbf{u}^{\text{int}} - \Delta t \left(\frac{1}{\Delta t} \nabla \cdot \mathbf{u}^{\text{int}} \right) \\ &= 0 \end{aligned}$$

or directly from (19).

A 3-cell flow



Eigenvalues of $\mathbf{F}$, $(\Delta t = 10^{-5})$



Periodic solutions

A solution $\mathbf{u}(t)$ is periodic if there exists a $\tau > 0$ such that $\mathbf{u}(t + \tau) = \mathbf{u}(t)$ for all $t \geq 0$. The minimal such τ is the period T .

Define the *flow* $\phi(\mathbf{u}_0, t)$ as the solution at time t with initial condition $\mathbf{u}(0) = \mathbf{u}_0$. We solve

$$\begin{pmatrix} \phi(\mathbf{u}, T) - \mathbf{u} \\ \psi(\mathbf{u}, T) \end{pmatrix} = \begin{pmatrix} \mathbf{0} \\ 0 \end{pmatrix}$$

via Newton's method for $\mathbf{u}^*(t)$ and period T , i.e., we solve

$$\begin{bmatrix} M^{(k)} - I & \phi_T^{(k)} \\ \psi_{\mathbf{u}}^{(k)} & \psi_T^{(k)} \end{bmatrix} \begin{pmatrix} \Delta \mathbf{u}^{(k)} \\ \Delta T^{(k)} \end{pmatrix} = - \begin{pmatrix} \mathbf{r}(\mathbf{u}^{(k)}, T^{(k)}) \\ \psi(\mathbf{u}^{(k)}, T^{(k)}) \end{pmatrix}$$

where M is the Jacobian matrix $\phi_{\mathbf{u}}$.

Let $\mathbf{u}^*(t)$ be one point on the periodic orbit. The stability of $\mathbf{u}^*(t)$ is determined by the eigenvalues of the *Monodromy matrix* $\phi_{\mathbf{u}}(\mathbf{u}^*)$, also known as the *Floquet multipliers*. The solution $\mathbf{u}^*(t)$ is stable if all the Floquet multipliers lie within the unit circle.

Applying the splitting (to M) as before, we solve

$$\begin{bmatrix} V_Q^T(M^{(k)} - I)V_Q & 0 & V_Q^T\phi_T^{(k)} \\ V_P^T M^{(k)} V_Q & V_P^T(M^{(k)} - I)V_P & V_P^T\phi_T^{(k)} \\ \psi_{\mathbf{u}}^{(k)} V_Q & \psi_{\mathbf{u}}^{(k)} V_P & \psi_T^{(k)} \end{bmatrix} \begin{pmatrix} \Delta \bar{\mathbf{q}}^{(k)} \\ \Delta \bar{\mathbf{p}}^{(k)} \\ \Delta T^{(k)} \end{pmatrix} = - \begin{pmatrix} V_Q^T \mathbf{r}(\mathbf{u}^{(k)}, T^{(k)}) \\ V_P^T \mathbf{r}(\mathbf{u}^{(k)}, T^{(k)}) \\ \psi(\mathbf{u}^{(k)}, T^{(k)}) \end{pmatrix}.$$

Repeating the previous system

$$\begin{bmatrix} V_Q^T(M^{(k)} - I)V_Q & 0 & V_Q^T\phi_T^{(k)} \\ V_P^T M^{(k)} V_Q & V_P^T(M^{(k)} - I)V_P & V_P^T\phi_T^{(k)} \\ \psi_{\mathbf{u}}^{(k)} V_Q & \psi_{\mathbf{u}}^{(k)} V_P & \psi_T^{(k)} \end{bmatrix} \begin{pmatrix} \Delta \bar{\mathbf{q}}^{(k)} \\ \Delta \bar{\mathbf{p}}^{(k)} \\ \Delta T^{(k)} \end{pmatrix} = - \begin{pmatrix} V_Q^T \mathbf{r}^{(k)} \\ V_P^T \mathbf{r}^{(k)} \\ \psi^{(k)} \end{pmatrix}.$$

Observe that

$$\mathbf{b}^* = \left. \frac{\partial \phi}{\partial T} \right|_{(\mathbf{u}^*, T^*)}$$

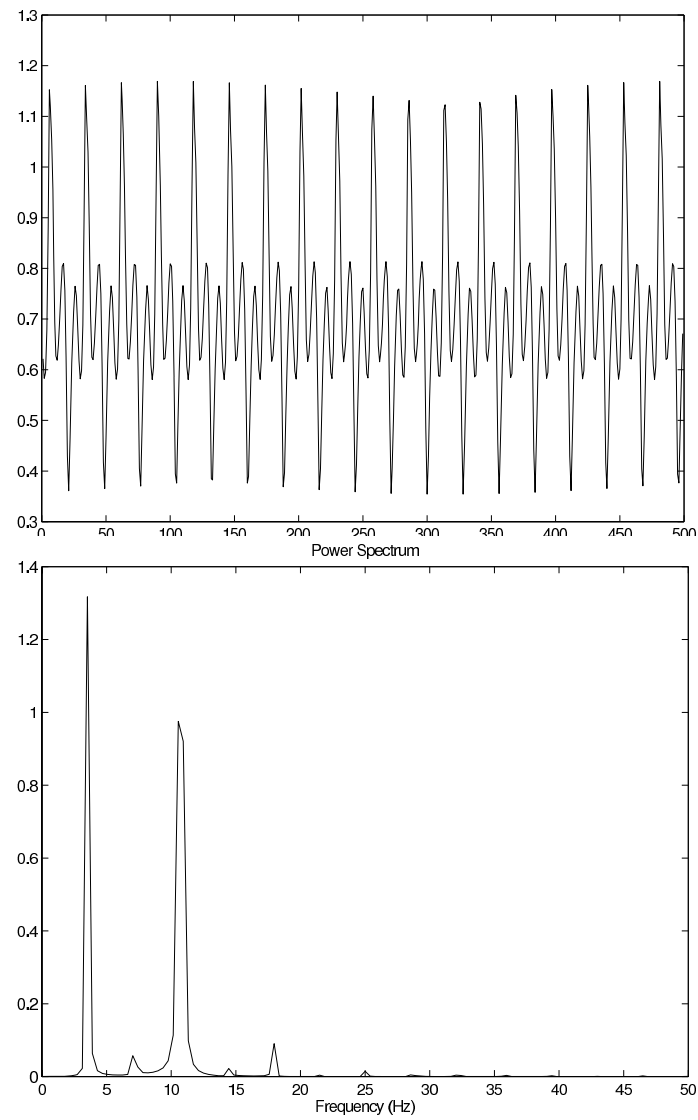
is an eigenvector of the Monodromy matrix corresponding to the eigenvalue one, thus $\mathbf{b}^* \in \mathcal{P}$ and $V_q^T \phi_T^{(k)}$ is small. We set to zero producing a block diagonal system.

Solve the Q -equations for $\Delta \bar{\mathbf{q}}^{(k)}$ as before and then the small system

$$\begin{bmatrix} V_P^T(M^{(k)} - I)V_P & V_P^T\phi_T^{(k)} \\ \psi_{\mathbf{u}}^{(k)} V_P & \psi_T^{(k)} \end{bmatrix} \begin{pmatrix} \Delta \bar{\mathbf{p}}^{(k)} \\ \Delta T^{(k)} \end{pmatrix} = - \begin{pmatrix} V_P^T \mathbf{r}^{(k)} + V_P^T M^{(k)} V_Q \Delta \bar{\mathbf{q}}^{(k)} \\ \psi^{(k)} + \psi_{\mathbf{u}}^{(k)} V_Q \Delta \bar{\mathbf{q}}^{(k)} \end{pmatrix}$$

by a direct method.

Bifurcation to flow on a torus



Implementation issues

1. The Chorin-Témam scheme is effectively a mapping of the velocity field only. (The pressure field is “slaved” to the velocity field.)
2. The action of the Jacobian was computed both by differencing and by solving the linearized problem.
3. We used ARPACK to perform the eigenvalue calculations (matrix free).
4. The eigenvalue clustering (around 1) increases the cost of the eigenvalue calculations.
5. We adopted a fixed basis size (due to eigenvalue clustering).
6. The eigenvalue clustering meant that the Q -equations (11) were poorly conditioned and needed to be solved with considerable accuracy since their solution appears in the RHS of the P equations.
7. The eigenvalue clustering meant that the power series (12) used to solve the Q -equations converged slowly.
8. Rather than solve iteratively, the matrices required for the Poisson solver were constructed and factored.
9. Arclength continuation comes at twice the cost. This is avoided when using direct methods as these require a single matrix factorization and two back solves.

Utility for the study of Taylor-Couette flow

Pros

- We observed good agreement with ENTWIFE calculations for steady bifurcation behavior (limit points, symmetry-breaking bifurcation points, Hopf bifurcation points) when the rotation rate of the outer cylinder was slow.
- We were able to compute unstable periodic orbits (unlike ENTWIFE).
- We could detect bifurcation to flow on a torus (unlike ENTWIFE).
- We could detect period doubling bifurcation (unlike ENTWIFE).

Cons

- Not particularly good agreement with ENTWIFE for strongly sheared flows. (We used a relatively coarse finite difference discretization.)

Is the Recursive Projection Method or Newton-Picard iteration for me?

- (Grey scale) Do you understand the black box well enough to identify the dependent and independent variables? If no, then STOP, otherwise continue
- (Resolution) Is $N < 1000$? If yes, then “RPM is for me”, otherwise proceed with caution
- (Stiffness) Is $\Delta t \geq 10^{-5}$? If yes, then “RPM may be for me” otherwise proceed with extreme caution
- (Cost) Is F is cheap to evaluate? If yes, then “RPM is just possibly for me”, otherwise STOP