A parallel framework for numerical bifurcation analysis in FreeFEM and its application to swirling jet flows

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Have you ever encountered an equation like this?

$$\mathcal{M}\frac{\partial \boldsymbol{q}}{\partial t} + \mathcal{R}\left(\boldsymbol{q}; \alpha, \beta, \ldots\right) = 0,$$

where

$\mathcal{M}$	mass matrix
$\mathcal{R}\left(\boldsymbol{q}; \alpha, \beta, \ldots\right)$	some nonlinear operator
$\boldsymbol{q}\left(\boldsymbol{x}, t\right)$	state vector
$\alpha, \beta, \ldots$	parameters.

How did you solve it?

$$\mathcal{M}\frac{\partial \boldsymbol{q}}{\partial t} + \mathcal{R}\left(\boldsymbol{q}; \alpha, \beta, \ldots\right) = 0$$

Time Integration

Finds solution ***trajectories***
as a function of time.

1. Choose a set of parameters.
2. Pick an initial condition.
3. "Shut up and calculate".
4. Change parameters/ICs and repeat.

Bifurcation Analysis

Finds solution ***manifolds***
as a function of parameters.

1. Choose an invariant state.
2. Continue state along parameter(s).
3. Search branch for bifurcations.
4. Change invariant state and repeat.

A typical numerical bifurcation analysis sequence

Start from an invariant state.

- Typically an equilibrium (fixed-point) solution.
- Usually found by Newton iteration.

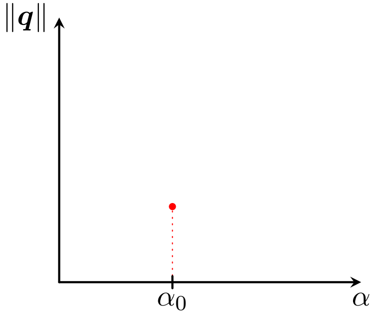

Figure: Bifurcation diagram

A typical numerical bifurcation analysis sequence

Start from an invariant state.

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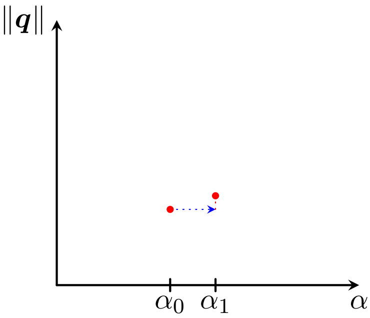
Trace state along parameter.

- Extend solution *point* along its solution *manifold*.
- Often performed via arclength continuation.



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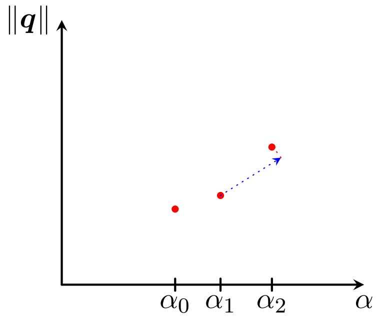

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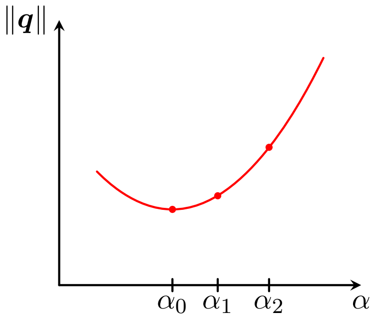

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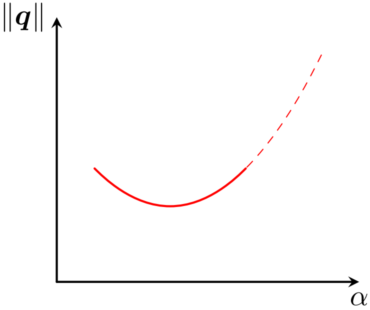
Compute linear stability of solution manifold.

- Identify bifurcation points along solution *manifold*.
- Generally done with eigenvalue computations.



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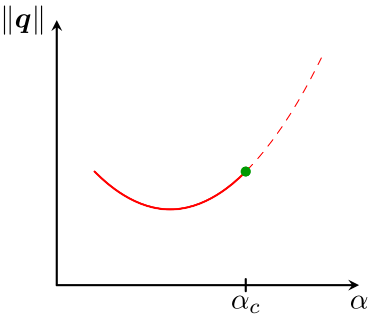

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- Generally done with eigenvalue computations.

Rinse, wash, repeat...

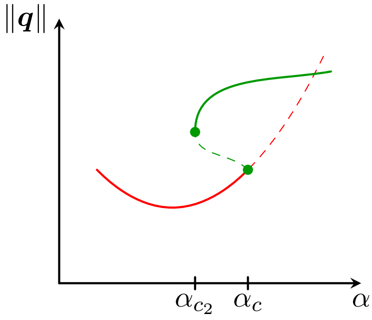

Figure: Bifurcation diagram

Large-scale bifurcation analysis

"Classic" numerical bifurcation tools

AUTO[1], MATCONT[2], etc.

- Dense systems of nonlinear ODE's.
- "Small" and "cheap" computations.
  - Typically $\boldsymbol{q} \sim O(1)$-$O(100)$ DoF.
- Can identify "complex" dynamics
  - e.g. limit cycles, connecting orbits, high codimension bifurcations, etc.

PDE-specific bifurcation analysis tools

LOCA (Trilinos)[3], pde2path (Matlab)[4]

- Sparse systems of nonlinear ODE's.
- "Large", "expensive" computations.
  - Typically $\boldsymbol{q} \sim O(10^4)$-$O(10^6)$ DoF.
- Mainly indentify "simple" dynamics
  - e.g. fixed-points and codimension-1 bifurcations.

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[1] https://github.com/auto-07p

[2] https://sourceforge.net/projects/matcont

[3] https://trilinos.github.io/

[4] https://www.staff.uni-oldenburg.de/hannes.uecker/pde2path/index.html

Outline

Objective

Develop a suite of generic routines leveraging FreeFEM and PETSc for scalable bifurcation analyses of nonlinear PDE's and PDE systems.

User provides:

1. Choice of finite element space
2. List of variable parameters
3. Variational forms of operators, including parameters
4. Macros/functions for specialized purposes (non-standard BC's, preconditioning, etc.)

Desired functionality:

1. Nonlinear solvers for equilibria, codimension-1,2 bifurcations, and periodic orbits.
2. Linear stability analysis for equilibria and periodic orbits.
3. Adaptive continuation schemes for equilibria, periodic orbits, and their bifurcations.
4. Organized file & mesh I/O, mesh adaptation, and pre- and post-processing.

An overview of the numerical approach

$$\mathcal{M}\frac{\partial \boldsymbol{q}}{\partial t} + \mathcal{R}\left(\boldsymbol{q}; \alpha, \beta, \ldots\right) = 0.$$

Identification of equilibrium solutions

$$\mathcal{R}\left(\boldsymbol{q}; \alpha, \beta, \ldots\right) = 0.$$

Directly achievable via `SNESSolve`[a] (see, newton-2d-PETSc.edp, for example.)

[a] `https://petsc.org/main/docs/manual/`

An overview of the numerical approach

$$\mathcal{M}\frac{\partial \boldsymbol{q}}{\partial t} + \mathcal{R}\left(\boldsymbol{q};\alpha,\beta,\ldots\right) = 0.$$

Identification of equilibrium solutions, $\boldsymbol{q}_e$

$$\mathcal{R}\left(\boldsymbol{q}_e;\alpha,\beta,\ldots\right) = 0.$$

Easy with PETSc `SNESSolve` (see, newton-2d-PETSc.edp, for example.)

Determination of the linear stability of equilibria

$$(\sigma + \mathrm{i}2\pi f)\mathcal{M}\hat{\boldsymbol{q}} + \left.\frac{\partial \mathcal{R}\left(\boldsymbol{q};\alpha,\beta,\ldots\right)}{\partial \boldsymbol{q}}\right|_{\boldsymbol{q}_e}\hat{\boldsymbol{q}} = 0.$$

Easy with SLEPc `EPSSolve` (see, navier-stokes-2d-SLEPc-complex.edp, for example.)

An overview of the numerical approach

Identification of equilibrium solutions, $\boldsymbol{q}_e$

$$\mathcal{R}\left(\boldsymbol{q}_e; \alpha, \beta, \ldots\right) = 0. \tag{1}$$

Easy with PETSc `SNESSolve` (see, newton-2d-PETSc.edp, for example.)

Determination of the linear stability of equilibria

$$(\sigma + \mathrm{i}2\pi f)\mathcal{M}\hat{\boldsymbol{q}} + \left.\frac{\partial \mathcal{R}\left(\boldsymbol{q}; \alpha, \beta, \ldots\right)}{\partial \boldsymbol{q}}\right|_{\boldsymbol{q}_e} \hat{\boldsymbol{q}} = 0. \tag{2}$$

Easy with SLEPc `EPSSolve` (see, navier-stokes-2d-SLEPc-complex.edp, for example.)

Identification of codimension-1 bifurcations of equilibria

Simultaneously satisfy (1) and (2) with $\sigma = 0$.

An overview of the numerical approach

Identification of codimension-1 bifurcation points of equilibria

Simultaneously satisfy (1) and (2) with $\sigma = 0$.

$$\left.\begin{aligned} \mathcal{R}\left(\boldsymbol{q}_e; \alpha, \beta, \ldots\right) &= 0 \\ \mathrm{i}2\pi f \mathcal{M}\hat{\boldsymbol{q}} + \left.\frac{\partial \mathcal{R}\left(\boldsymbol{q}; \alpha, \beta, \ldots\right)}{\partial \boldsymbol{q}}\right|_{\boldsymbol{q}_e} \hat{\boldsymbol{q}} &= 0, \\ \|\hat{\boldsymbol{q}}\| &= 1. \end{aligned}\right\} \Rightarrow \overbrace{\mathcal{R}^{\star}\left(\boldsymbol{q}_e, \hat{\boldsymbol{q}}, f; \alpha, \beta, \ldots\right)}^{\text{Augmented operator}} = 0.$$

Solved with PETSc `SNESSolve` (exploiting block Schur decomposition)

An overview of the numerical approach

Identification of codimension-1 bifurcation points of equilibria

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Solved with PETSc `SNESSolve` (exploiting block Schur decomposition)

A similar augmentation approach can be used to solve systems describing all other dynamics.
(e.g. identification of periodic orbits; continuation of equilibria, periodic orbits, and local bifurcations)

For more details of a less general case, see:

C. Douglas, Chapter 2, *Dynamics of swirling jets and flames*, Ph.D. Thesis. Georgia Institute of Technology. 2021.

Implementation progress...

Current functionality:

1. Nonlinear fixed-point solvers:
   - Done: equilibria, codimension-1 bifurcations of equilibria, periodic orbits.
   - To-do: codimension-1 bifurcations of periodic orbits, codimension-2 bifurcations.
2. Linear analysis:
   - Done: stability of equilibria (also resolvent, adjoint, and structural sensitivity of equilibria).
   - To-do: stability of periodic orbits.
3. Adaptive continuation schemes:
   - Done: equilibria, codimension-1 bifurcations of equilibria, periodic orbits.
   - To-do: codimension-1 bifurcations of periodic orbits, codimension-2 bifurcations.
4. Other items:
   - To-do: Improvements to code structure & workflow, smoother integration with mesh adaptation.

If you are interested in progress updates or co-developing: chris.douglas@ladhyx.polytechnique.fr

Outline

What is a swirling jet?

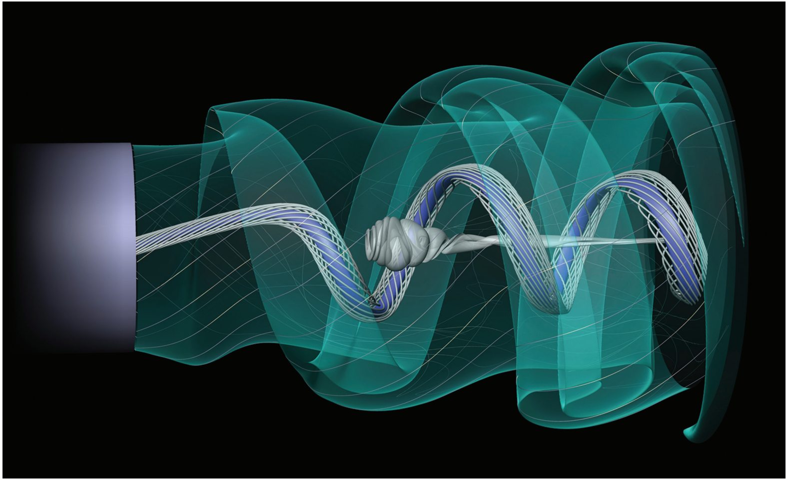
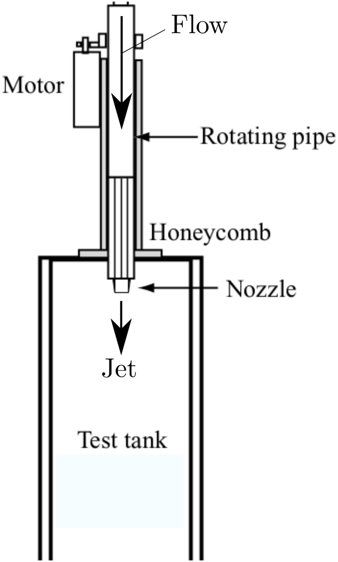


Figure: Petz et al. *Phys. Fluids*, 2011.

Experimental Demonstration (Liang & Maxworthy, *JFM*, 2005)

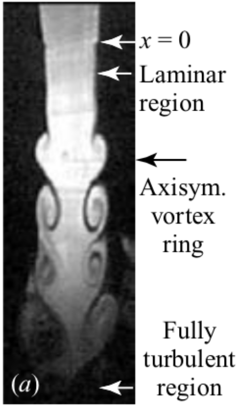
Qualitative evolution with increasing swirl ratio S

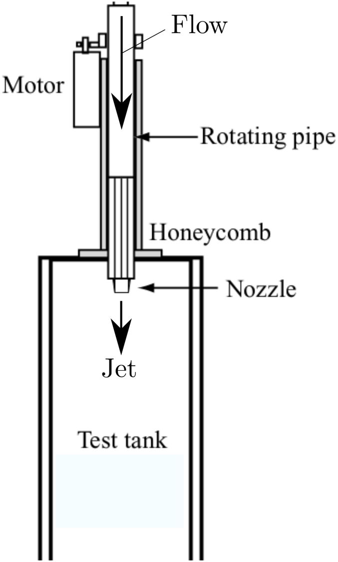


Experimental Demonstration (Liang & Maxworthy, *JFM*, 2005)

Qualitative evolution with increasing swirl ratio S

$S = 0$: **axisymmetric** straight jet





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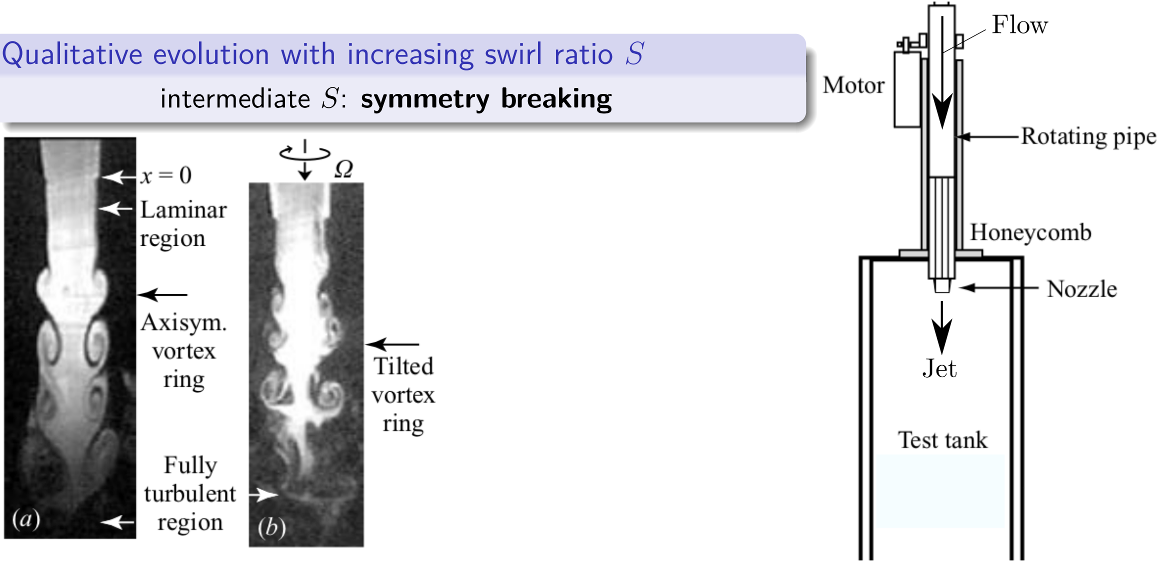
Qualitative evolution with increasing swirl ratio S

intermediate S: **symmetry breaking**



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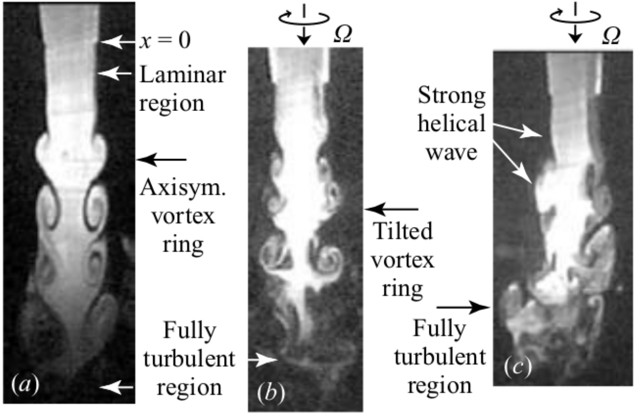
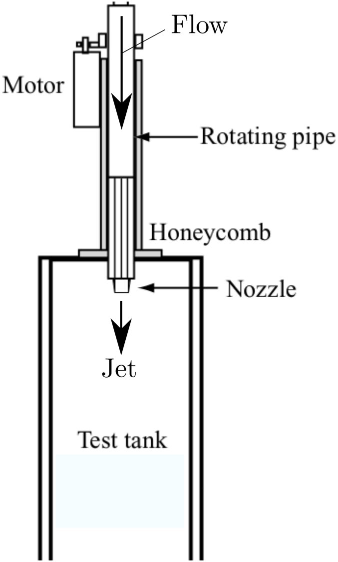
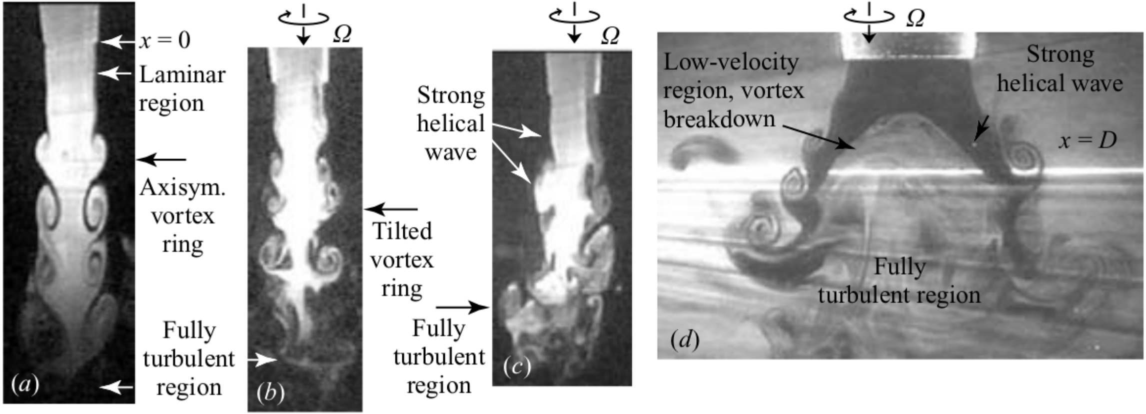




Experimental Demonstration (Liang & Maxworthy, *JFM*, 2005)

Qualitative evolution with increasing swirl ratio S

intermediate S: **symmetry breaking** high S: "**vortex breakdown**"



Flow Configuration

Incompressible Navier–Stokes equations cast in cylindrical domain $(\boldsymbol{q}(x, r, \theta, t) = (\boldsymbol{u}, p)^{\mathrm{T}})$.

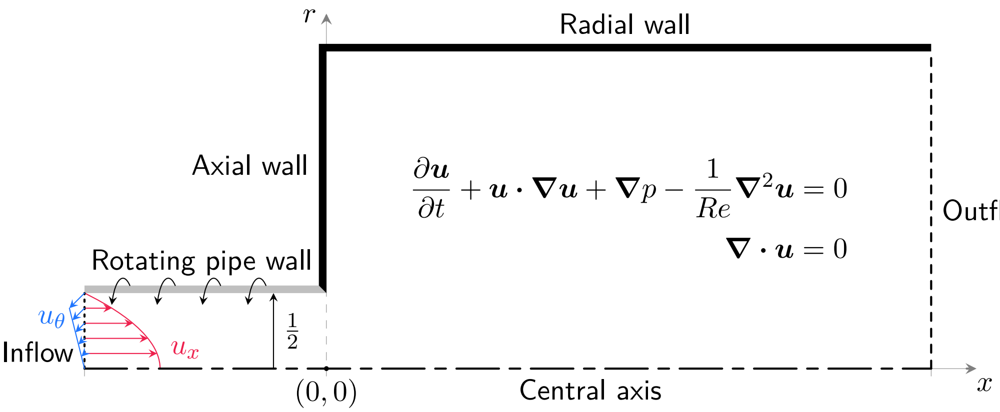


Figure: Meridional plane schematic of the axisymmetric system.

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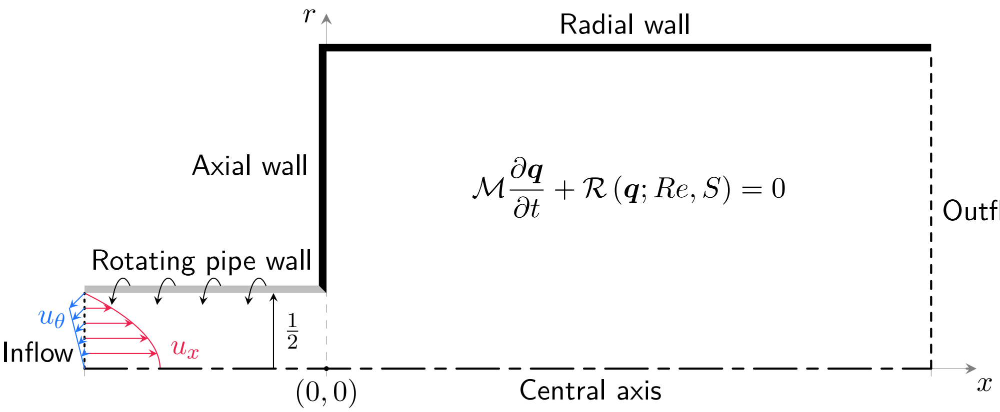
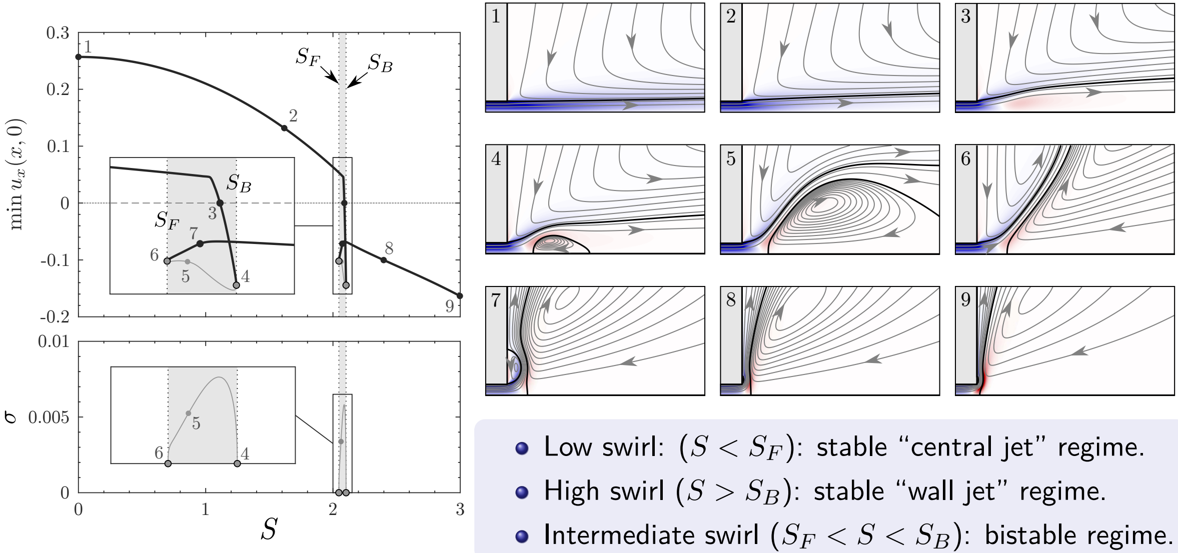


Figure: Meridional plane schematic of the axisymmetric system.

Example Results: Multistability of steady, axisymmetric swirling jet states



- Low swirl: $(S < S_F)$: stable "central jet" regime.
- High swirl $(S > S_B)$: stable "wall jet" regime.
- Intermediate swirl $(S_F < S < S_B)$: bistable regime.

Example Results: Multistability of steady, axisymmetric swirling jet states

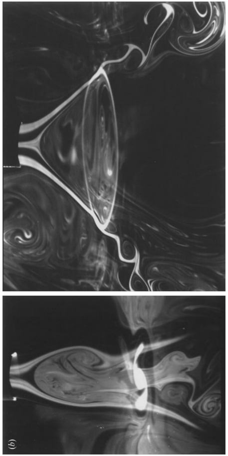
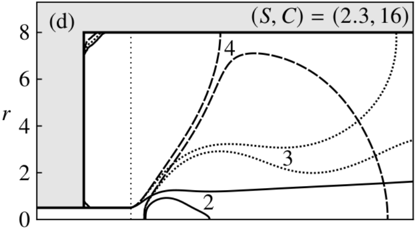


Figure: Billant, Chomaz, & Huerre, *JFM*, 1998.



- Dynamical model agrees with experiments.
- Approach enables a precise, rigorous analysis of the bistable mechanics.

For more details, see:

Douglas & Lesshafft, Confinement effects in laminar swirling jets, *J. Fluid Mech.* **945**, 2022. doi: 10.1017/jfm.2022.589.

Example Results: Symmetry breaking in swirling jets

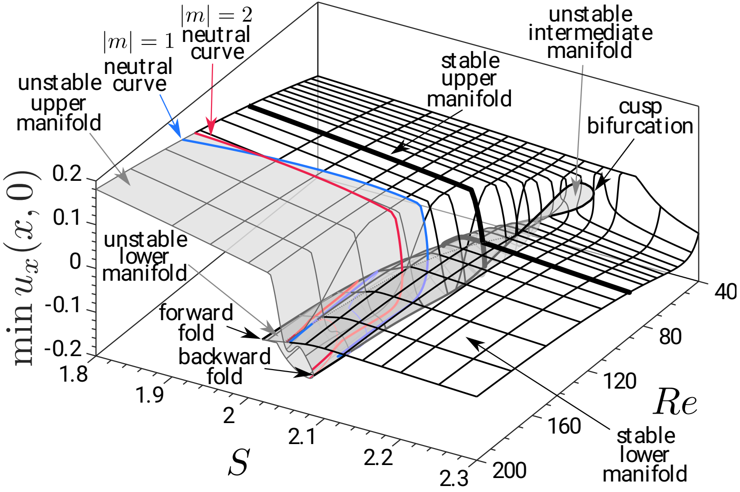
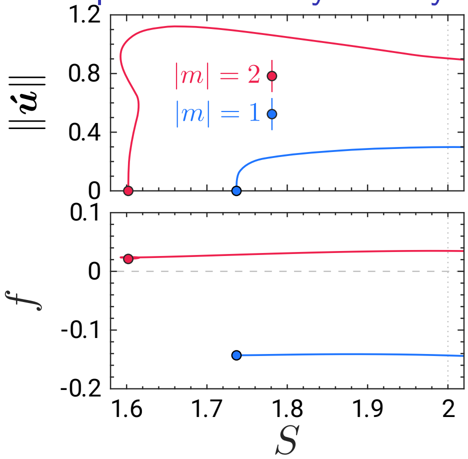


Figure: Visualization of the steady solution manifold over the Re–S plane.

Example Results: Symmetry breaking in swirling jets

$|m| = 2$



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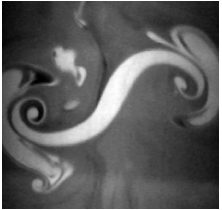

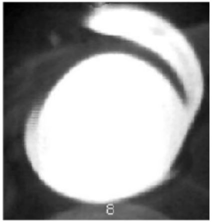

$|m| = 1$

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(Exp. vis. from Loiseleux & Chomaz, *Phys. Fluids*, 2003.)

For more details, see:

Douglas, Emerson, & Lieuwen, Nonlinear dynamics of fully developed swirling jets, *J. Fluid Mech.* **924**, 2021. doi: 10.1017/jfm.2021.615

Summary

- A generic FreeFEM/PETSc-based bifurcation analysis framework for nonlinear PDE's.
  - Solvers for identifying fixed points, bifurcations (fold, pitchfork, Hopf), and periodic orbits.
  - Adaptive parametric branch continuation methods.
  - Linear analysis methods (stability, adjoint, structural sensitivity, resolvent, etc.)
- An example application of this framework to study the dynamics of swirling jet flows.
  - Steady branch continuation used to elucidate bistable behaviors.
  - Bifurcation analysis to investigate symmetry breaking phenomena.

For more details...

- C. Douglas, *Dynamics of swirling jets and flames*, Ph.D. Thesis. Georgia Institute of Technology. 2021.
- C. Douglas, B. Emerson, & T. Lieuwen, Nonlinear dynamics of fully developed swirling jets, *J. Fluid Mech.* **924**, 2021.
- C. Douglas, B. Emerson, & T. Lieuwen, Dynamics and bifurcations of laminar annular swirling and non-swirling jets, *J. Fluid Mech.* **943**, 2022.
- C. Douglas & L. Lesshafft, Confinement effects in laminar swirling jets, *J. Fluid Mech.* **945**, 2022.

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