

A variational framework for flow optimization: an introduction to adjoints

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recap: time-periodic flow

$$\frac{d}{dt}q = L(t)q \qquad \qquad L(t+T) = L(t) \qquad \text{period T}$$
 with the formal solution
$$q(t) = A(t)q_0 \text{ initial condition}_{\text{propagator}}$$

from periodicity
$$A(t+T) = A(t) A(T) = A(t) C$$

$$q_n = C \ q_{n-1} = C^n \ q_0$$

monodromy matrix (mapping over one period)

initial state

recap: time-periodic flow

Example: pulsatile channel flow



recap: time-periodic flow

Example: pulsatile channel flow



time-periodic and generally time-dependent flow

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pseudo-Floquet analysis adjoint analysis

Example: pulsatile channel flow

Can we analyze the amplification of energy between one period, i.e., for a non-periodic system matrix ?

We have

$$\frac{d}{dt}q = L(t)q$$

with the formal solution

 $q(t) = A(t) q_0$ initial condition final solution propagator

time-periodic and generally time-dependent flow



pseudo-Floquet analysis adjoint analysis

Example: pulsatile channel flow

We can formulate the optimal amplification of energy as

$$\begin{aligned} G(t)^2 &= \max_{q_0} \frac{\langle q, q \rangle}{\langle q_0, q_0 \rangle} \\ &= \max_{q_0} \frac{\langle A(t)q_0, A(t)q_0 \rangle}{\langle q_0, q_0 \rangle} \\ &= \max_{q_0} \frac{\langle A^H(t)A(t)q_0, q_0 \rangle}{\langle q_0, q_0 \rangle} \end{aligned}$$

time-periodic and generally time-dependent flow



pseudo-Floquet analysis adjoint analysis

Example: pulsatile channel flow

$$G(t)^{2} = \max_{q_{0}} \frac{\langle A^{H}(t)A(t)q_{0}, q_{0} \rangle}{\langle q_{0}, q_{0} \rangle}$$

 $A^H A$ is a **normal** matrix

 \Rightarrow the maximum is achieved for the principal eigenvector of A^HA

the principal eigenvector (and eigenvalue) can be found by power iteration

$$q_0^{(n+1)} = \rho^{(n)} A^H A q_0^{(n)}$$

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Example: pulsatile channel flow

$$q_0^{(n+1)} = \rho^{(n)} A^H A q_0^{(n)}$$

break the power iteration into two pieces

$$w(t) = A q_0^{(n)}$$

first step

propagation of initial condition forward in time

time-periodic and generally time-dependent flow



pseudo-Floquet analysis adjoint analysis

Example: pulsatile channel flow

$$q_0^{(n+1)} = \rho^{(n)} A^H A q_0^{(n)}$$

break the power iteration into two pieces

$$q_0^{(n+1)} = \rho^{(n)} A^H(t) w(t)$$

second step

propagation of final condition backward in time

time-periodic and generally time-dependent flow



pseudo-Floquet analysis adjoint analysis

Example: pulsatile channel flow







A can be any discretized solution operator. The above technique (adjoint looping) can be applied to general time-dependent stability problems.

time-periodic and generally time-dependent flow

Example: pulsatile channel flow

applying adjoint looping to the pulsatile (inter-period) stability problem







time-periodic and generally time-dependent flow



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reformulate the optimal growth problem variationally

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we wish to optimize

$$J = \frac{\|q\|^2}{\|q_0\|^2} \to \max$$

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1.1

subject to the constraint

$$\frac{d}{dt}q - Lq = 0$$

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pseudo-Floquet analysis adjoint analysis

rather than substituting the constraint directly into the cost functional ...

$$J = \frac{\|q\|^2}{\|q_0\|^2} = \frac{\|\exp(tL)q_0\|^2}{\|q_0\|^2} \to \max$$
$$\frac{d}{dt}q - Lq = 0 \quad \text{only valid for LTI systems}$$
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time-periodic and generally time-dependent flow



pseudo-Floquet analysis adjoint analysis

... we enforce the equation via a Lagrange multiplier $\,\widetilde{q}\,$

$$J = \frac{\|q\|^2}{\|q_0\|^2} - \left\langle \tilde{q}, \left(\frac{d}{dt}q - Lq\right) \right\rangle \to \max$$

This has the advantage that the solution to the governing equation does not have to be known *explicitly*.

Other constraints (such as initial and boundary conditions) can be added.

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pseudo-Floquet analysis adjoint analysis

for an optimum we have to require all first variations of J to be zero

$$J = \frac{\|q\|^2}{\|q_0\|^2} - \left\langle \tilde{q}, \left(\frac{d}{dt}q - Lq\right) \right\rangle \to \max$$
$$\frac{\delta J}{\delta \tilde{q}} = 0 \quad \Leftrightarrow \quad \left\langle \delta \tilde{q}, \left(\frac{d}{dt}q - Lq\right) \right\rangle = 0$$
$$\frac{\delta J}{\delta q} = 0 \quad \Leftrightarrow \quad \left\langle \tilde{q}, \left(\frac{d}{dt}\delta q - L\delta q\right) \right\rangle = 0$$

 δJ

 $\delta \tilde{q}$

time-periodic and generally time-dependent flow



pseudo-Floquet analysis adjoint analysis

for an optimum we have to require all first variations of J to be zero

$$J = \frac{\|q\|^2}{\|q_0\|^2} - \left\langle \tilde{q}, \left(\frac{d}{dt}q - Lq\right) \right\rangle \to \max$$

$$\frac{d}{dt}q - Lq = 0$$

 $\frac{\delta J}{\delta q} = 0 \quad \Rightarrow \quad \left\langle \tilde{q}, \left(\frac{d}{dt} \delta q - L \ \delta q \right) \right\rangle = 0$

time-periodic and generally time-dependent flow



pseudo-Floquet analysis adjoint analysis

for an optimum we have to require all first variations of J to be zero

$$J = \frac{\|q\|^2}{\|q_0\|^2} - \left\langle \tilde{q}, \left(\frac{d}{dt}q - Lq\right) \right\rangle \to \max$$
$$\frac{J}{\tilde{q}} = 0 \quad \rightleftharpoons \quad \frac{d}{dt}q - Lq = 0$$

 $\frac{\delta J}{\delta q} = 0 \quad \Rightarrow \quad \left\langle \left(-\frac{d}{dt} \tilde{q} - L^H \tilde{q} \right), \delta q \right\rangle = 0$

 δJ

 $\delta \tilde{q}$

 δJ

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pseudo-Floquet analysis adjoint analysis

for an optimum we have to require all first variations of J to be zero

$$J = \frac{\|q\|^2}{\|q_0\|^2} - \left\langle \tilde{q}, \left(\frac{d}{dt}q - Lq\right) \right\rangle \to \max$$

$$\frac{d}{dt}q - Lq = 0$$

direct problem

$$-\frac{d}{dt}\tilde{q} - L^H\tilde{q} = 0$$

adjoint problem

KKT-condition

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pseudo-Floquet analysis adjoint analysis

adjoint variables can be interpreted as sensitivities

$$J = \text{obj} - \left\langle \tilde{q}, \left(\frac{d}{dt}q - Lq \right) \right\rangle \to \max$$

let us add an external body force to the governing equations

$$\frac{d}{dt}q - Lq = f$$

$$\delta J = -\langle \tilde{q}, \delta f \rangle$$

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pseudo-Floquet analysis adjoint analysis

adjoint variables can be interpreted as sensitivities

$$J = \text{obj} - \left\langle \tilde{q}, \left(\frac{d}{dt}q - Lq \right) \right\rangle \to \max$$

let us add an external body force to the governing equations



$$\nabla_f J = -\tilde{q}$$

sensitivity to external body force

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pseudo-Floquet analysis adjoint analysis

Example: which adjoint variable measures the sensitivity to a mass source/sink?

$$J = \text{obj} - \langle \tilde{\mathbf{u}}, NS(\mathbf{u}) \rangle -$$

 $\langle \xi,
abla \cdot \mathbf{u}
angle$

enforcing momentum conservation

enforcing mass conservation





time-periodic and generally time-dependent flow



pseudo-Floquet analysis adjoint analysis

Example: which adjoint variable measures the sensitivity to a mass source/sink?

$$J = \text{obj} - \langle \tilde{\mathbf{u}}, NS(\mathbf{u}) \rangle$$

enforcing momentum conservation

 $-\langle \xi,
abla \cdot \mathbf{u}
angle$

enforcing mass conservation

assuming a mass source/sink

•
$$\mathbf{u} = Q$$
 $\delta J = \langle \boldsymbol{\xi}, \delta Q \rangle$
adjoint pressure = sensitivity to a mass source/sink



Sensitivity to internal changes (changes of specific eigenvalues with respect to parameter variations)

general formulation

$$A(p)q = \lambda Bq$$
 p Reynolds number Re wave number α, β base-flow $U(y)$

perturbation expansion

 $(A + \delta A)(q + \delta q) = (\lambda + \delta \lambda)B(q + \delta q)$

Sensitivity to internal changes (changes of specific eigenvalues with respect to parameter variations)

general formulation

$$(A + \delta A)(q + \delta q) = (\lambda + \delta \lambda)B(q + \delta q)$$

$$(A - \lambda B)q + (A - \lambda B)\delta q + (\delta A - \delta \lambda B)q + (\delta A - \delta \lambda B)\delta q = 0$$

$$\approx 0$$

(higher order)

Sensitivity to internal changes (changes of specific eigenvalues with respect to parameter variations)

general formulation

$$(A + \delta A)(q + \delta q) = (\lambda + \delta \lambda)B(q + \delta q)$$

$$(A - \lambda B)\delta q + (\delta A - \delta \lambda B)q \approx 0$$

Sensitivity to internal changes (changes of specific eigenvalues with respect to parameter variations)

general formulation

$$(A - \lambda B)\delta q + (\delta A - \delta \lambda B)q \approx 0$$

Itsee adjoint $q^+(A - \lambda B) = 0 \iff (A^+ - \lambda^* B^+)q^+ = 0$

$$q^{+}(A - \lambda B) \delta q + q^{+}(\delta A - \delta \lambda B) q \approx 0$$

Sensitivity to internal changes (changes of specific eigenvalues with respect to parameter variations)

general formulation

$$A(p)q = \lambda Bq$$

perturbation expansion

gradient

Example: sensitivity to a scalar parameter

complex Ginzburg-Landau

$$u_t = \underbrace{\left(-\mathcal{D}\partial_x + \gamma\partial_{xx} + \mu(x)\right)}_{A} u_{\nu} = U + 2ic_u$$

$$\Rightarrow \nabla_U A = -\partial_x$$

eigenvalue sensitivity

 $\nabla_U \lambda = \tilde{u}^+ \nabla_U A \tilde{u}$

 $A\tilde{u} = \lambda \tilde{u}$ $A^{+}\tilde{u}^{+} = \lambda^{*}\tilde{u}^{+}$ $\lambda = \sigma + i\omega$

 $= -\tilde{u}^+ \partial_x \tilde{u}$

Example: sensitivity to a scalar parameter

complex Ginzburg-Landau
$$u_{t} = \underbrace{\left(-\mathcal{D}\partial_{x} + \gamma\partial_{xx} + \mu(x)\right)}_{\nu = U + 2ic_{u}} u$$
$$= U + 2ic_{u} A$$
$$\Rightarrow \nabla_{U}A = -\partial_{x} \qquad \begin{vmatrix} A\tilde{u} = \lambda\tilde{u} \\ A^{+}\tilde{u}^{+} = \lambda^{*}\tilde{u}^{+} \\ A^{+}\tilde{u}^{+} = \lambda^{*}\tilde{u}^{+} \\ \lambda = \sigma + i\omega \end{vmatrix}$$
eigenvalue sensitivity
$$\nabla_{U}\lambda = \tilde{u}^{+}\nabla_{U}A\tilde{u} \qquad \begin{vmatrix} A\tilde{u} = \lambda\tilde{u} \\ A^{+}\tilde{u}^{+} = \lambda^{*}\tilde{u}^{+} \\ \lambda = \sigma + i\omega \end{vmatrix}$$
$$\nabla_{U}\sigma = \operatorname{Real}(\nabla_{U}\lambda) \qquad \nabla_{U}\omega = \operatorname{Imag}(\nabla_{U}\lambda)$$

sensitivity of growth rate

sensitivity of frequency

Sensitivity to internal changes (changes of specific eigenvalues with respect to parameter variations)

Example: choose base flow profile as control variable

$$\nabla_{\mathbf{U}}\lambda = -(\nabla\mathbf{u})^H\tilde{\mathbf{u}} + \nabla\tilde{\mathbf{u}}\cdot\mathbf{u}^*$$

$$p_{\substack{\text{wave number } \alpha \\ \text{base-flow } U(y)}}$$

relate mean flow modification to small control forces

delay onset of instabilities to higher Reynolds numbers; increase stability margins

Flow chart for sensitivity/receptivity analysis






Generalizations Example: flow around a cylinder base flow calculation LNS adjoint LNS (power iteration) adjoint modes global modes receptivity sensitivity 12_{1} ٥<mark>ل</mark> **L** $\tilde{u}_{ m adjoint}$ $\tilde{v}_{\mathrm{adjoint}}$ EPTT, Sao Paulo, Sept. 2012



Example: flow around a cylinder



$u_{\text{wavemaker}}$



$v_{\rm wavemaker}$







What if the operator perturbation is stochastic?

$$\frac{d}{dt}q - Lq = 0$$

$$L(t) = L_S + \epsilon \mu(t)S$$
statistically steady part uncertain part stochastic process $d\mu = -\nu \mu dt + dW$

 \mathcal{V} ~ auto-correlation time

What if the operator perturbation is stochastic?

We have to describe the solution statistically: propagation of covariance (second-order moments)

$$K = \mathcal{E}(qq^H)$$

evolution equation for the covariance matrix (expansion of propagator A(t))

$$\frac{d}{dt}K = (L_S + \epsilon^2 SD)K + K(L_S + \epsilon^2 SD)^H + \epsilon^2 (SKD + DKS^H)$$

with
$$D = \int_0^t \exp(\tau L_s) S \exp(-\tau L_S) \exp(-\nu \tau) d\tau$$

stochastic channel flow (perturbed base flow profile) $\,
u = 1/5 \, \epsilon = 0.2 \,$





nonlinear Navier-Stokes equations

How does this affect the adjoint looping ?







For long-time integrations and high-dimensional problems we quickly reach the limits of storage devices.



optimized checkpointing

store flow fields at coarse intervals ••• and use as initial conditions for repeated forward integrations

no checkpointing (store everything)



no checkpointing (store everything)



no checkpointing (store everything)























We often have governing equations with auxiliary evolution equations (e.g., for eddy-viscosity), but these auxiliary variables may not be part of the cost objective.

$$q = \begin{pmatrix} \mathbf{u} \\ \nu_t \end{pmatrix} \qquad \frac{d}{dt} \begin{pmatrix} \mathbf{u} \\ \nu_t \end{pmatrix} = \begin{pmatrix} \mathbf{f}(\mathbf{u}, \nu_t) \\ g(\nu_t, \ldots) \end{pmatrix} \overset{\text{governing}}{\underset{\text{model}}{\text{model}}}$$

This leads to *semi-norm* constraints.

$$\|\mathbf{q}\|\equiv\|\mathbf{u}\|$$
 We can have $\|\mathbf{q}\|=0$ with $\,\mathbf{q}
eq\mathbf{0}$

not a true norm

→ causes singularities (non-convergence)

We need additional constraints to avoid singularities.

- constrained variational approach (penality terms)
- → optimization on hyper-spheres



Is the 2-norm appropriate for all applications ? Can we consider a worst-case scenario ?



localization of the optimal structures, symmetry breaking (work in progress)













multiple inhomogeneous directions/complex geometry



$$q_{k} = L q_{k-1}$$

for $j = 1 : k - 1$
$$H_{j,k-1} = \langle q_{j}, q_{k} \rangle$$

$$q_{k} = q_{k} - H_{j,k-1} q_{j}$$

end
$$H_{k,k-1} = ||q_{k}||$$

$$q_{k} = q_{k}/H_{k,k-1}$$

only multiplications by L are necessary

 \implies eig{L} \approx eig{H}














Arnoldi algorithm (a Krylov subspace technique) to compute the Hessenberg matrix H





Summary

A variational approach for fluid stability problems provides a flexible and effective framework that allows the treatment time-invariant, time-periodic, time-dependent, linear and nonlinear problems.

- Adjoint variables can be interpreted as carriers of gradient/ sensitivity information to external driving terms.
- Weighted (scalar) products of direct and adjoint variables yield structural sensitivity information and can be used for complex flow optimizations or the influence analysis of particular terms in the governing equations.
- Semi-norm constraints and p-norm extensions add even more flexibility.