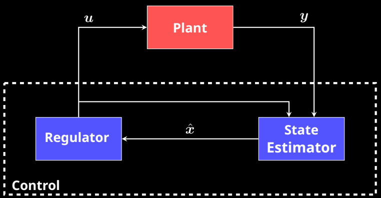
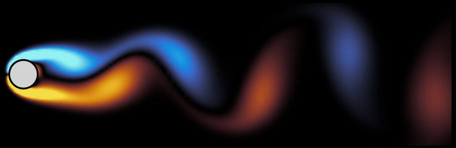




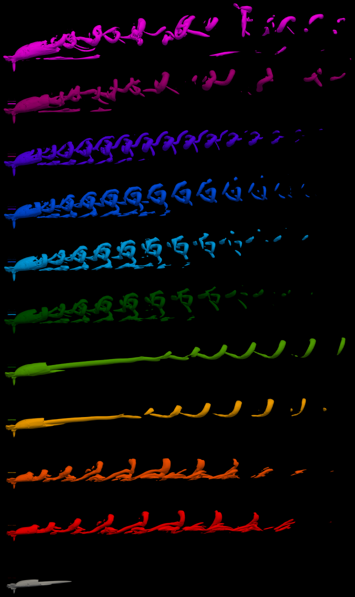
Time-stepping approach to large-scale linear algebra

Jean-Christophe Loiseau

Ricardo Frantz

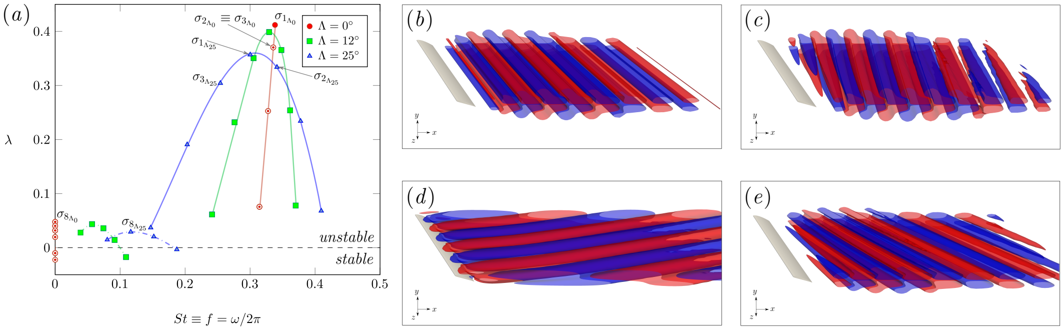
Jean-Christophe Loiseau

Jean-Christophe Robinet



Hydrodynamic stability : Set of tools to investigate the first stages of transition to turbulence.

Primarily a numerical linear algebra issue for large-scale dynamical systems such as discretized PDEs.


(a)
$\sigma_{2_{\Lambda_0}} \equiv \sigma_{3_{\Lambda_0}}$
$\sigma_{1_{\Lambda_0}}$
$\sigma_{1_{\Lambda_{25}}}$
$\sigma_{3_{\Lambda_{25}}}$
$\sigma_{2_{\Lambda_{25}}}$
$\sigma_{8_{\Lambda_0}}$
$\sigma_{8_{\Lambda_{25}}}$
$\Lambda = 0°$
$\Lambda = 12°$
$\Lambda = 25°$
λ
unstable
stable
$St \equiv f = \omega/2\pi$
0
0.1
0.2
0.3
0.4
0.5
(b)
(c)
(d)
(e)

Dynamics $f : \mathbb{R} \times \mathbb{R}^n \times \mathbb{R}^p \to \mathbb{R}^n$

$$\dot{\mathbf{X}} = \boxed{f}\left(t, \boxed{\mathbf{X}}, \boldsymbol{\mu}\right)$$

State vector $\mathbf{X} \in \mathbb{R}^n$

Flow map $\varphi_\tau : \mathbb{R}^n \times \mathbb{R}^p \to \mathbb{R}^n$

$$\mathbf{X}_{k+1} = \boxed{\varphi_\tau}(\mathbf{X}_k, \boldsymbol{\mu})$$

How to compute fixed points or periodic orbits of the system and study their linear stability properties given only a time-stepper ?

Fixed points

Continuous time

$$f(\mathbf{X}, \boldsymbol{\mu}) = \mathbf{0}$$

Discrete time

$$\varphi_\tau(\mathbf{X}, \boldsymbol{\mu}) - \mathbf{X} = \mathbf{0} \quad \forall \tau$$

Linearized system

Continuous time

$$\dot{\mathbf{x}} = \boxed{\mathbf{L}}\,\mathbf{x}$$

Jacobian matrix $\in \mathbb{R}^{n\times n}$

Discrete time

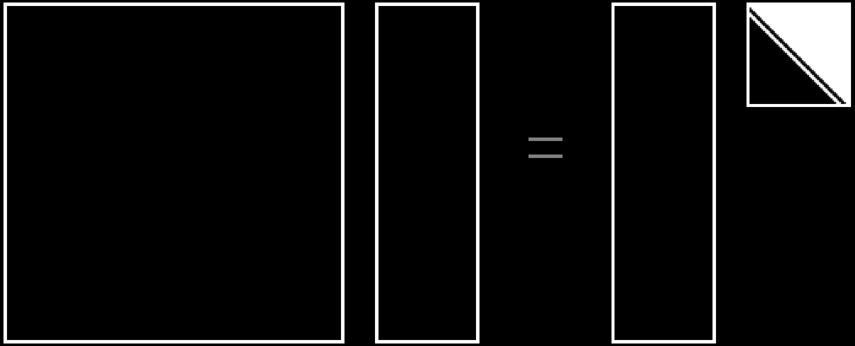
$$\mathbf{x}_{k+1} = \boxed{\exp(\tau\mathbf{L})}\,\mathbf{x}_k$$

Exponential Propagator $\in \mathbb{R}^{n\times n}$

Arnoldi factorization

Alexei Krylov

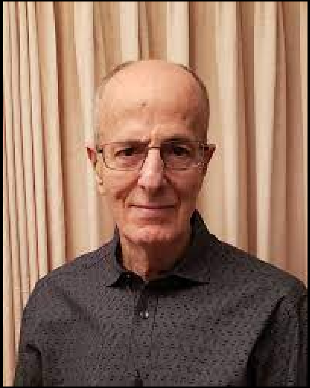
Cornelius Lanczos



Generalized Minimal Residual Method

Require: $\mathbf{x}_0$, $\mathbf{A}$, $\mathbf{b}$
Ensure: $\|\mathbf{A}\mathbf{x} - \mathbf{b}\|_2^2 \le \varepsilon$

```
r ← b − A x_0
q_1 ← r / ||r||_2
for k = 1, 2, ··· do
    y ← A q_k
    for j = 1, 2, ··· , k do
        h_jk ← q_j^T y
        y ← y − h_jk q_j
    end for
    hk + 1, k = ||y||_2
    q_{k+1} = y / h_{k+1,k}
    minimize ||Hc − e_1 ||r||_2||_2
    x_k ← x_0 + Q_k c
end for
```



Youssef Saad

Fixed point computation

$$\mathcal{F}(\mathbf{X}, \boldsymbol{\mu}) \equiv \varphi_{\tau}\left(\mathbf{X}, \boldsymbol{\mu}\right) - \mathbf{X} = \mathbf{0}$$

$$\mathbf{J} \equiv \exp\left(\tau \mathbf{L}\right) - \mathbf{I}$$

Newton-GMRES solver for fixed point computation

Require: $\mathbf{X}$
Ensure: $\|\mathbf{F}(\mathbf{X})\| \leq \varepsilon$
  $\mathbf{r} \leftarrow \mathcal{F}(\mathbf{X}_0)$
  while $\|\mathbf{r}\| \geq \varepsilon$ **do**
    $\delta\mathbf{x} \leftarrow \mathrm{gmres}(\mathbf{F}', \mathbf{r})$
    $\mathbf{X} \leftarrow \mathbf{X} + \delta\mathbf{x}$
    $\mathbf{r} \leftarrow \mathbf{F}(\mathbf{X})$
  end while

- The product $\exp(\tau \mathbf{L})\,\mathbf{x}$ can easily be computed with a time-stepper.
- Good performances even without preconditionning!
- Extension to periodic orbits is straightforward.

Espen Åkervik

Selective Frequency Damping

Filter's gain

$$\dot{\mathbf{X}} = f(t, \mathbf{X}, \boldsymbol{\mu}) - \boxed{\chi}\,(\mathbf{X} - \mathbf{Y})$$
$$\dot{\mathbf{Y}} = \boxed{\omega_c}\,(\mathbf{X} - \mathbf{Y})$$

Filter's cutoff frequency

BoostConv

Corrected state

$$\boxed{\tilde{\mathbf{x}}_{t+1}} = \boxed{\mathbf{x}_{t+1}} - \mathbf{Y}\mathbf{Y}^{\dagger}\left(\mathbf{x}_{t+1} - \tilde{\mathbf{x}}_t\right) + \mathbf{X}\mathbf{Y}^{\dagger}\left(\mathbf{x}_{t+1} - \tilde{\mathbf{x}}_t\right)$$

Predicted state

Vincenzo Citro

Standard test case in the incompressible hydrodynamic stability community. Here, we solve it with the spectral element solver `Nek5000` + `nekStab`.

- From $Re = 40 \quad \rightarrow \quad Re = 70$.
- 2000 spectral elements.
- 3^{rd} order-accurate EXT/BDF scheme.
- Helmholtz solver tolerance set to 10^{-12}.
- Pressure Poisson solver tolerance set to 10^{-10}.

Coarse mesh : $32\,000$ grid points with $\Delta t = 0.025$

	SFD	**BootConv**	**Newton-GMRES**	**Newton-GMRES** (dyn. tol.)
Time	42 s	30 s	65 s	30 s
RAM Usage	0.3 Gb	0.4 Gb	1.8 Gb	0.5 Gb

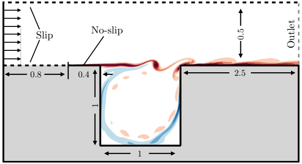
Intermediate mesh : $72\ 000$ grid points with $\Delta t = 0.01$

	SFD	**BootConv**	**Newton-GMRES**	**Newton-GMRES** (dyn. tol.)
Time	230 s ($\times 6$)	235 s ($\times 8$)	370 s ($\times 6$)	230 s ($\times 8$)
RAM Usage	0.3 Gb	0.4 Gb	1.8 Gb	0.8 Gb

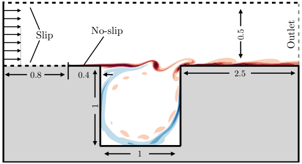
Fine mesh : $128\,000$ grid points with $\Delta t = 0.005 =$

	SFD	**BootConv**	**Newton-GMRES**	**Newton-GMRES** (dyn. tol.)
Time	884 s ($\times 3.8$)	1260 s ($\times 5$)	1370 s ($\times 3.7$)	774 s ($\times 3.6$)
RAM Usage	0.4 Gb	0.6 Gb	2.9 Gb	0.8 Gb

Another relatively standard test-case for flow control and reduced-order modeling[a]. A branch of discrete eigenvalues eventually become unstable.



[a] Merci Denis !



- From $Re = 4000 \quad \rightarrow \quad Re = 4500$.
- 4000 spectral elements.
- 3rd order-accurate EXT/BDF scheme.
- Helmholtz solver tolerance set to 10^{-12}.
- Pressure Poisson solver tolerance set to 10^{-10}.

Coarse mesh : $64\,000$ grid points with $\Delta t = 0.0025$

	SFD	**BootConv**	**Newton-GMRES**	**Newton-GMRES** (dyn. tol.)
Time	975 s	1600 s	600 s	400 s
RAM Usage	0.3 Gb	0.4 Gb	1.8 Gb	0.5 Gb

Intermediate mesh : $144\,000$ grid points with $\Delta t = 0.001$

	SFD	**BootConv**	**Newton-GMRES**	**Newton-GMRES** (dyn. tol.)
Time	3120 s ($\times 3.2$)	NA	500 s ($\times 1$)	400 s ($\times 1$)
RAM Usage	0.4 Gb		1.8 Gb	0.8 Gb

Fine mesh : $256\ 000$ grid points with $\Delta t = 0.0006$

	SFD	**BootConv**	**Newton-GMRES**	**Newton-GMRES** (dyn. tol.)
Time	10^4 s ($\times 3.5$)	NA	1900 s ($\times 3.8$)	1500 s ($\times 3.8$)
RAM Usage	0.6 Gb		2.9 Gb	0.8 Gb

$$
\begin{aligned}
\exp(\tau \mathbf{L}) - \mathbf{I} &\simeq (\mathbf{I} + \tau \mathbf{L}) - \mathbf{I} \\
&\propto \mathbf{L}
\end{aligned}
$$

$$\mathrm{spec}(\mathbf{L}) \in \mathcal{D} = \{z : \mathrm{Re}(z) \leq -\delta\}$$

$$\mathrm{spec}(\mathbf{J}) \in \mathcal{D}' = \{z : |z+1| \leq \exp(-\tau\delta)\}$$

The residual ε after k iterations can be upper bounded by

$$\varepsilon \leq \kappa(\mathbf{V}) \exp(-k\tau\delta)$$

with $\kappa(\mathbf{V})$ the condition number of the eigenbasis.

The number of iterations k needed to reach a given tolerance ε is given by

$$k \leq \frac{1}{\tau\delta} \log\left(\frac{\kappa(\mathbf{V})}{\varepsilon}\right).$$

This bound is however overly pessimistic. If p eigenvalues are unstable, $\mathcal{O}(p)$ extra iterations are needed.

Linear stability analyses

Spectral decomposition

$$\exp(\tau \mathbf{L})\,\mathbf{v} = \mathbf{v}\mu$$

- Matrix-vector product computed with a time-stepper.
- Eigenvalues of interest already have the largest magnitude.
- No other spectral transformation needed for fast convergence of iterative solvers.

Krylov subspace dimension : 128

Mesh	*Coarse*	*Intermediate*	*Fine*
# of conv. ev.	2	2	2
Time	30 s	210 s	800 s

Krylov subspace dimension : 192

Mesh	*Coarse*	*Intermediate*	*Fine*
# of conv. ev.	4	10	10
Time	54 s	324 s	1140 s

Krylov subspace dimension : 256

Mesh	*Coarse*	*Intermediate*	*Fine*
# of conv. ev.	6	10	10
Time	80 s	418 s	1520 s

Suppose μ_i is an isolated eigenvalue such that the rest of the spectrum is enclosed in the disk

$$\mathcal{D} = \{z : |z - c| < \rho\},$$

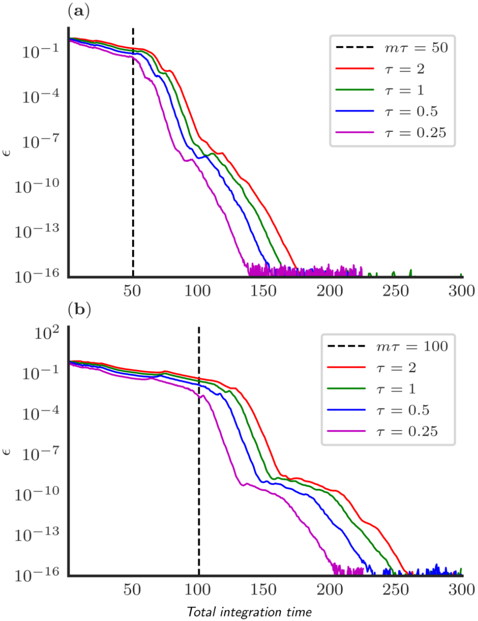
i.e. a disk centered in c and of radius ρ.

Upper bound for the residual ε_i associated to μ_i after a k-step Arnoldi factorization is given by

$$\varepsilon_i \leq \kappa(\mathbf{V}) \left(\frac{\rho}{|\mu_i - c|} \right)^k .$$

The further apart μ_i is from the rest of the spectrum, the faster it converges.

- The larger τ, the larger the gap between μ_i and the rest of the spectrum.
- The larger τ, the fewer iterations are needed to converge the leading eigenspectrum.
- The larger τ, the more expensive each matrix-vector product is.



For a random starting vector, the number of Krylov iterations before convergence is proportional to the flow-through time.

Adjoint sensitivity analysis

Adjoint operator

$$\langle \mathbf{y} | \mathbf{L}\mathbf{x} \rangle = \langle \mathbf{L}^{\dagger}\mathbf{y} | \mathbf{x} \rangle$$

Sensitivity to baseflow modification

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

Sensitivity to a steady force

$$\nabla_{\mathbf{F}}\lambda = \mathbf{U}^{\dagger}$$

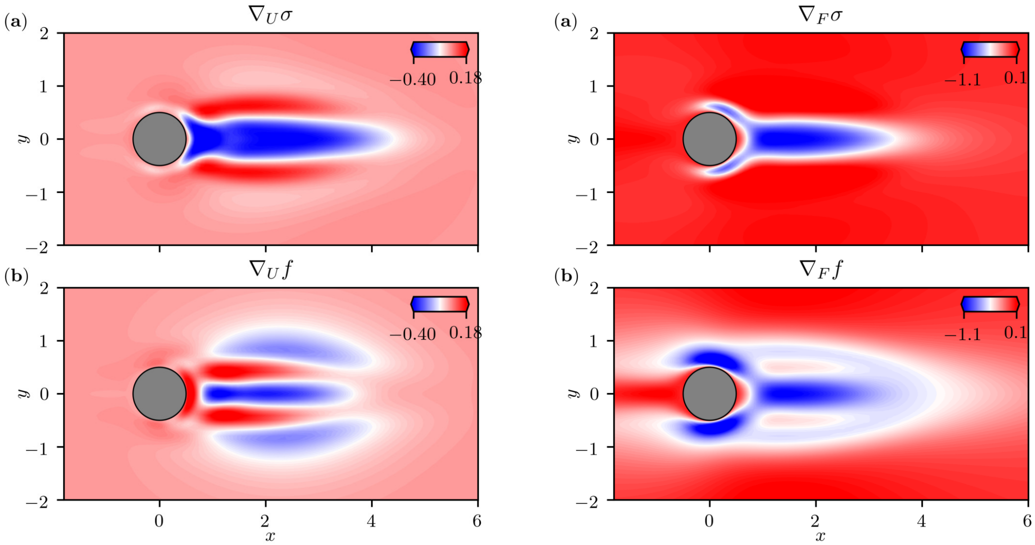
$$\Updownarrow$$

$$\mathbf{L}^{\dagger}\mathbf{U}^{\dagger} = \nabla_{\mathbf{U}}\lambda$$

$$\dot{\mathbf{x}} = \mathbf{L}^{\dagger}\mathbf{x} + \mathbf{b}$$

$$\mathbf{x}(\tau) = \exp\left(\tau \mathbf{L}^{\dagger}\right)\mathbf{x}_0 + \int_0^{\tau} \exp\left((\tau - t)\mathbf{L}^{\dagger}\right) \mathbf{b} \, \mathrm{d}t$$

$$\left(\mathbf{I} - \exp\left(\tau \mathbf{L}^{\dagger}\right)\right) \mathbf{x} = \int_0^{\tau} \exp\left((\tau - t)\mathbf{L}^{\dagger}\right)\mathbf{b} \, \mathrm{d}t$$


(a)
$\nabla_U \sigma$
(a)
$\nabla_F \sigma$
(b)
$\nabla_U f$
(b)
$\nabla_F f$
-0.40 0.18
-1.1 0.1
x
y

What’s next ?

- Linear optimal perturbation analysis is a straightforward extension with the operator being

$$\mathbf{A} = \exp\left(\tau \mathbf{L}^\dagger\right) \exp(\tau \mathbf{L}).$$

- Resolvent analysis can also be cast in this framework although it requires being a bit more careful.

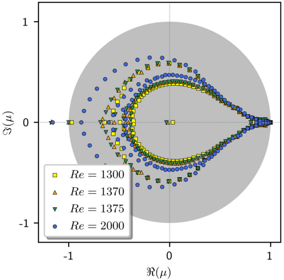
$$\begin{aligned} \underset{\mathbf{x}}{\text{maximize}} \quad & \|\exp(\tau \mathbf{L})\mathbf{x}\|^2_{\mathbf{W}} \\ \text{subject to} \quad & \|\mathbf{x}\|^2_{\mathbf{W}} = 1 \end{aligned}$$

- Extension to compute (unstable) periodic orbits, satisfying

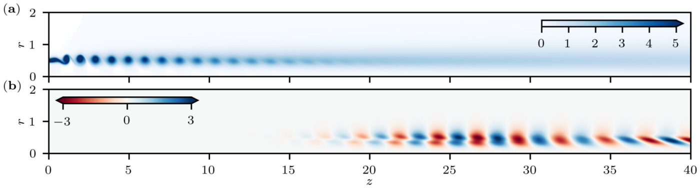
$$\mathbf{X} - \varphi_\tau(\mathbf{X}) = 0 \quad \text{for} \quad \tau = k\tau^*$$

  is also straightforward.

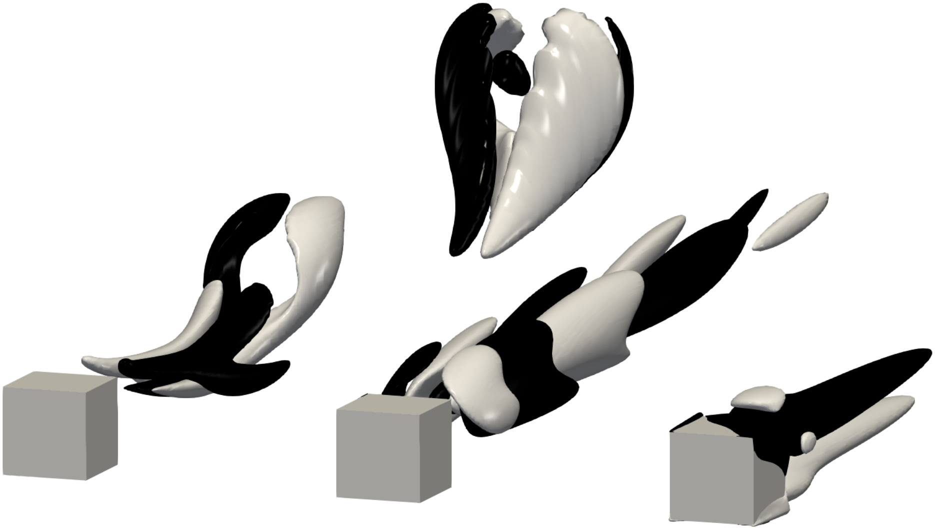
- The same applies to computing the eigenvalues of the monodromy matrix for Floquet analysis.



1
0
-1
-1
0
1
$\Im(\mu)$
$\Re(\mu)$
$Re = 1300$
$Re = 1370$
$Re = 1375$
$Re = 2000$



(a)
(b)
r
0
1
2
0
1
2
3
4
5
−3
0
3
0
5
10
15
20
25
30
35
40
z



Quantitative comparison of the matrix-forming vs. time-stepper approaches using the exact same solver is still lacking.

If you have some extra $$$ to use for this, please be my guest. You know how to get in touch with me !

https://loiseaujc.github.io/

https://loiseau-jc.medium.com/

@loiseau_jc

Thank you for your attention!

Any question?