Spectral structures for nonlinear operators towards applications

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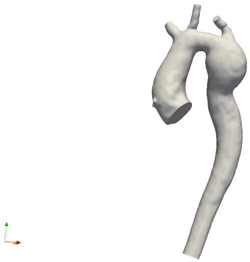
Outline

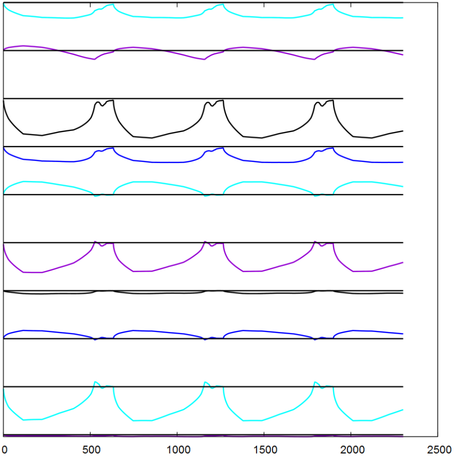
Motivation: blood flow in aorta



- simulation of bloodflow in an aorta
- courtesy http://www.mevis.de/ Andreas Ruopp / HLRS

Motivation: blood flow in aorta

signals [u,v,w] for aortic-blood-flow shown for every 164 step 1:10 / 51



- 3 velocity components at different locations of the aorta in a sequence of time steps
- 3dim signals at 2735 nodes in total
- 2301 time steps
- signals 1–10 are shown
- understood as a vector of signals
- signals have a common timewise behaviour
- data from simulation
- courtesy http://www.mevis.de/ Andreas Ruopp / HLRS

decomposing sequences

- Given is a bounded sequence $k \mapsto g_k$

$$\begin{bmatrix} g_0 & g_1 & \cdots & g_k & \cdots & g_n \end{bmatrix}$$

  of states, measurements, iterations or discretization steps. These are typically produced by a nonlinear (discretization) operator, which should produce stable results in a compact domain.
- The target is to find an **approximating** sequence $\tilde{g}_k$ of the g_k of the type

$$\tilde{g}_k = \sum_{l=0}^{n} v_l \ \lambda_l^k \quad \forall \ k \in \mathbb{N}_{\mathbf{0}} \tag{1}$$

  for some complex values λ_l and the time step k.
- this is the sum of vector valued coefficients multiplied by powers given by the timestep k of λ_l, e.g. vectors in the (finite dimensional) state space of a discretization of a partial differential equation.
- Even if all g_k might be real vectors, λ_l and v_l are complex. But for all exist conjugate complex counterparts as part of the sum. The terms $v_l \ \lambda_l^k + \overline{v_l} \ \overline{\lambda_l}^k$ are relevant.
- Some of these λ_l may approximate eigenvalues of the Koopman-operator. Therefore we name these eigenvalues. The vectors v_l are named Koopman-modes.

properties of eigenvalues

- The eigenvalues are properties of the (discretization) operator and not simple properties of the iteration sequence.
  $\Rightarrow$ for a stable operator the eigenvalues are restricted to $|\lambda_l| \leq 1$.
- We found a numerical procedure resulting in approximations of the eigenvalues forcing the modulus of the eigenvalues not to exceed 1.
- There are other eigenvalues with $|\lambda_l| \ll 1$. These eigenvalues are typically inaccurate in the numerical approximation and depend on different parameters. A member vector $v_l \lambda_l^k$ will disappear exponentially for $k \longrightarrow \infty$ if $|\lambda_l| < 1$ even if $\|v_l\|$ is large.
- Important is to find the correct elements $v_l \lambda_l^k$ for $|\lambda_l| = 1$. These Koopman-modes will survive with increasing time step k. They deliver the long term instationary behaviour of the iteration sequence.
- If the error of the procedure is small, the future iterations of the sequence can be predicted.

what is to be solved

- We determine a vector c with the property

$$G_{j:p+j}\ c = \begin{bmatrix} g_{0+j} & g_{1+j} & g_{2+j} & \dots & g_{p+j} \end{bmatrix} \begin{bmatrix} c_0 \\ c_1 \\ c_2 \\ \vdots \\ c_p \end{bmatrix} \approx 0 \tag{2}$$

  for $j = 0, 1, \cdots, n-p$ (generalizing DMD by Peter Schmidt). The vector c is not unique.
- Understood as the coefficient vector of a polynom c will have a polynom degree p smaller than the number of measurements n.
- We will not discuss here, what ≈ 0 means. This question leads to the approximation by $\widetilde{g}_k$ for g_k.

meaning and significance of vector c

- Essential for the whole procedure is the determination of the vector c defining the eigenvalues as roots of the associated polynom.
- The Koopman-modes v_l can be calculated by knowledge solely of the eigenvalues λ_l and the iteration sequence G.
- The larger the degree $p \leq n$ of the approximating polynom c is, the smaller the approximation error. But it can be shown, that the quality of being a Koopman-eigenvalue is getting worse.
- We can show how Koopman-eigenfunctions can be derived from the representation.

how to get the Koopman-modes?

- For the root λ_l divide the polynom c by the linear factor $\begin{bmatrix} -\lambda_l \\ 1 \end{bmatrix}$

$$c = w_l * \begin{bmatrix} -\lambda_l \\ 1 \end{bmatrix} \quad \forall\, l = 1, \cdots, p \tag{3}$$

- Use the polynom coefficient vector w_l to build the vectors v_l

$$v_l = \tilde{G}_{0:p-1} \frac{w_l}{w_l(\lambda_l)} \tag{4}$$

- The Koopman-modes v_l define the sum

$$\begin{bmatrix} \tilde{g}_0 & \tilde{g}_1 & \dots & \tilde{g}_n \end{bmatrix} = \sum_{l=1}^{\mathbf{p}} v_l \left[1, \lambda_l, \lambda_l^2, \dots, \lambda_l^{\mathbf{n}}\right] \tag{5}$$

- The matrix of measurements $\tilde{G}_{0:p-1}$ could even be replaced by a matrix of other measurements related to the problem.

matrices to be investigated

- Determine a polynom coefficient vector c by

$$\widehat{G}\; c = \begin{bmatrix} g_{0+0} & g_{4+0} & g_{8+0} & \cdots & g_{4q+0} \\ g_{0+1} & g_{4+1} & g_{8+1} & \cdots & g_{4q+1} \\ g_{0+2} & g_{4+2} & g_{8+2} & \cdots & g_{4q+2} \\ g_{0+3} & g_{4+3} & g_{8+3} & \cdots & g_{4q+3} \end{bmatrix} c \overset{?}{\approx} 0 \qquad (6)$$

- The polynom coefficient vector $c = \begin{bmatrix} c_0 & c_1 & \ldots & c_q \end{bmatrix}$ defines a polynom

$$c\,(\lambda) = \sum_{k=0}^{q} c_k \left(\lambda^4\right)^k \qquad (7)$$

  This polynom has q coefficients and q primary roots μ_l each defining 4 different roots by solving $\mu_{lj} = \lambda_{lj}^4$ for $j = 1, 2, 3, 4$.
- This approach reduces the number of involved roots and the size of the polynom by a factor of (here) 4.
- We have still to take the 4-th root of the calculated root and the related mode.
- Using instead of 4 another number allows for handling of a large number of time steps.

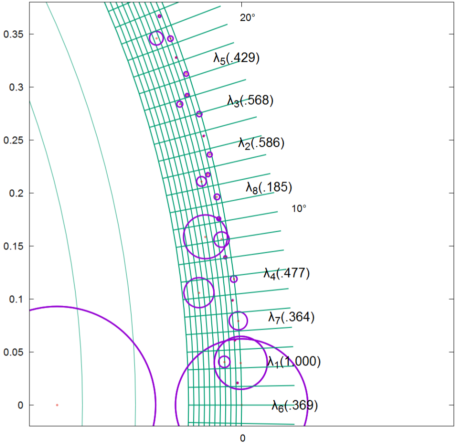
An example of Koopman modes in the flow across an aorta

- An approximation of the complete unsteady trajectory is given by $k \mapsto Re \sum_l v_l \lambda_l^k$.
- Shown are animations the time behaviour of the Koopman-modes $k \mapsto \mathrm{Re}\, v_l \lambda_l^k$ for $k = 0, \cdots, 130$
- The selected 8 Koopman-modes have maximal value for $\|v_l \lambda_l^{k_{max}}\|$ at the last (!) time step k_{max}.
- They are ordered by the angle of the complex number λ_l given by $arg(\lambda_l) = \mathrm{Im} \log \lambda_l \; l = 1, 2, \cdots, 8$
- All the animations show smooth fields.
- The different Koopman-modes are obviously related to different domains.
- As the frequency $arg(\lambda_l)$ is getting larger, the movement is faster.
- It can be seen, that $arg(\lambda_l) \; l = 2, \cdots, 8$ are multiples of $arg(\lambda_6)$. The theory of the Koopman-operator is suggesting this.
- The first case for λ_6 is constant, because it is related to $\lambda = 1$.

Other remarks for the pictures

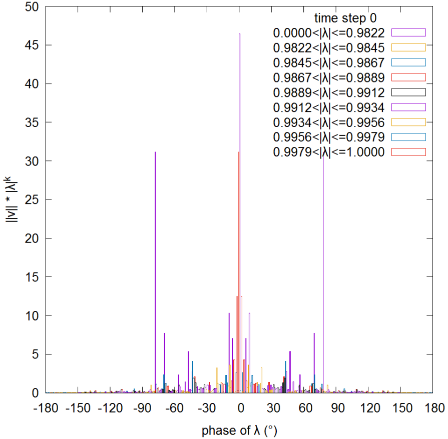
- The region shown is only a part of the simulated domain of the aorta.
- The vector fields $\mathrm{Re}\, v_l \lambda_l^k$ have no common scaling in the pictures.
- Not all time steps are shown to limit the size of the PDF-file.

most important eigenvalues and Koopman-modes



- A fraction of the unit circle is shown.
- Eigenvalues λ_l near 1 with weights $\|v_l\|$ of the Koopman modes proportional to diameter of the blue circles.
- the values λ_l $l = 1, 2, \cdots, 8$ ordered with respect to the size of their modes at the last defined step.
- The relative weights are given by in $\lambda(\cdots)$

norm of modes $\|v_l \lambda_l^k\|$ decreasing with time k



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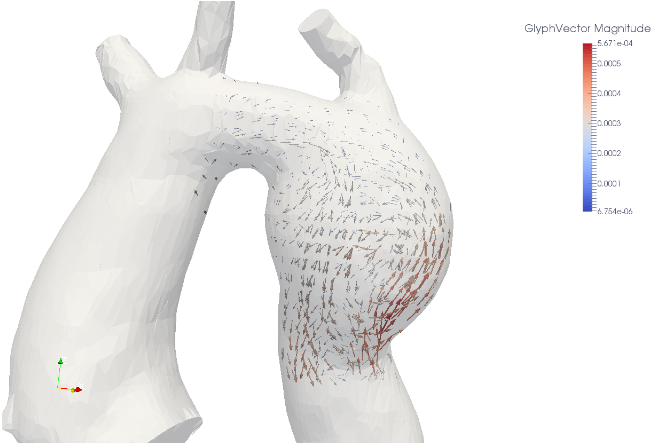
- The animation shows how modes $\|v_l \lambda_l^k\|$ behave in dependency on $|\lambda_l|$.
- Modes with $|\lambda_l| < 1$ disappear along the trajectory.
- Modes with $|\lambda_l| = 1$ remain. They are important for the long term behaviour.
- Modes with $|\lambda_l| > 1$ would be unstable. They would indicate an unstable iteration operator.

HLRS

1- constant Koopman-mode 6

$|\lambda_6| = 1.0000 \; arg(\lambda_6) = 0.0000 \; rel.norm = 0.369$



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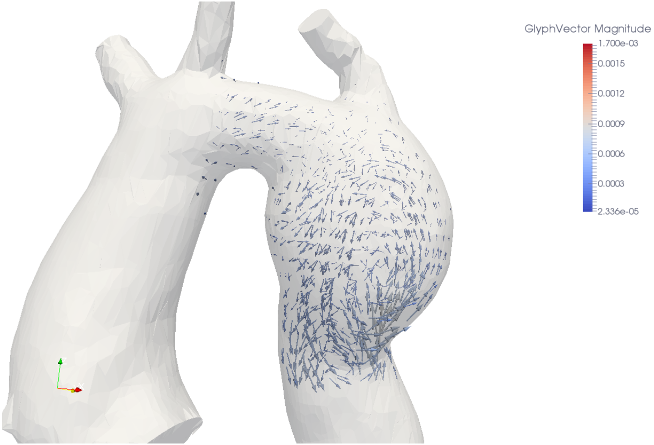
2- Koopman-mode 1

$$|\lambda_1| = 1.0000 \ arg(\lambda_1) = 2.2765 \approx 1 \ x \ arg(\lambda_6) \ rel.norm = 1.00$$



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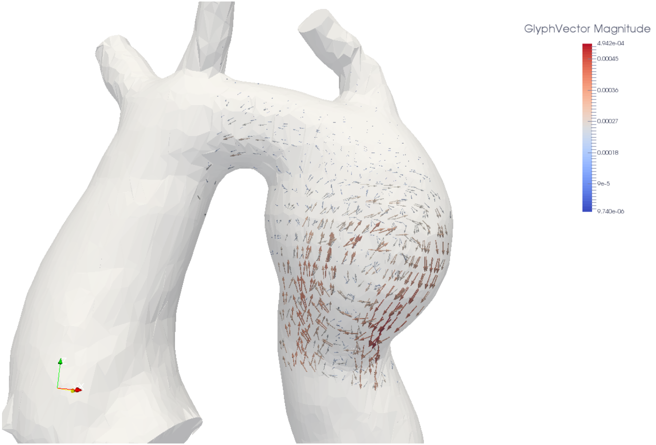
3- Koopman-mode 7

$|\lambda_7| = 0.99999 \; arg(\lambda_7) = 4.5522 \approx 2 \; x \; arg(\lambda_6) \; rel.norm = 0.364$



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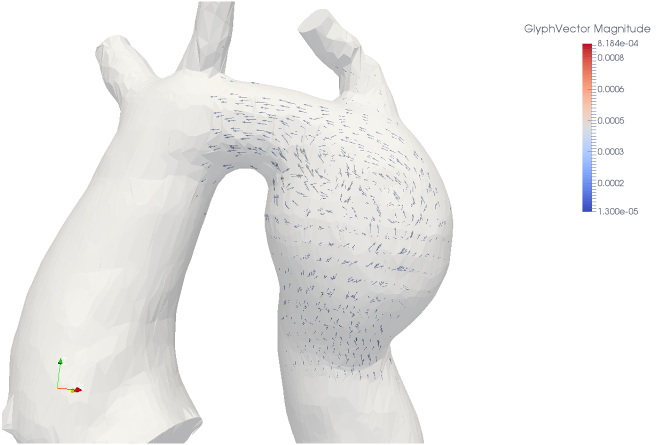
4- Koopman-mode 4

$$|\lambda_4| = 0.99969 \; arg(\lambda_4) = 6.8267 \approx 3 \; x \; arg(\lambda_6) \; rel.norm = 0.477$$



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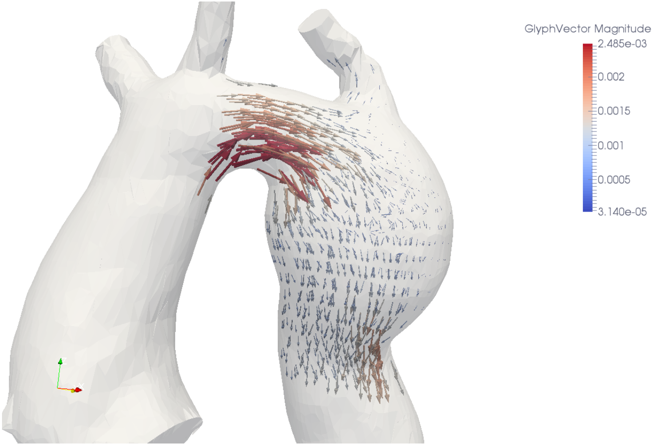
5- Koopman-mode 8

$$|\lambda_8| = 0.99631 \; arg(\lambda_8) = 11.362 \approx 5 \; x \; arg(\lambda_6) \; rel.norm = 0.185$$



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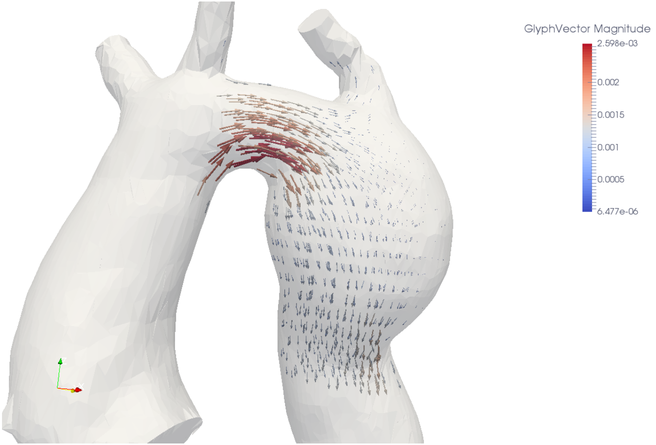
6- Koopman-mode 2

$|\lambda_2| = 0.99830 \ arg(\lambda_2) = 13.685 \approx 6 \ x \ arg(\lambda_6) \ rel.norm = 0.586$



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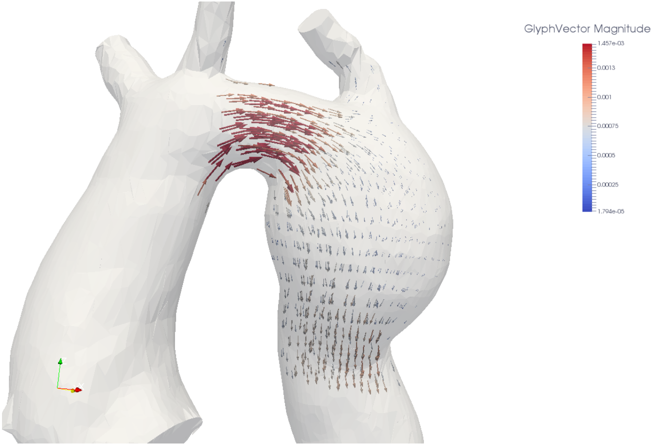
7- Koopman-mode 3

$|\lambda_3| = 0.99856 \ arg(\lambda_3) = 15.950 \approx 7 \ x \ arg(\lambda_6) \ rel.norm = 0.568$



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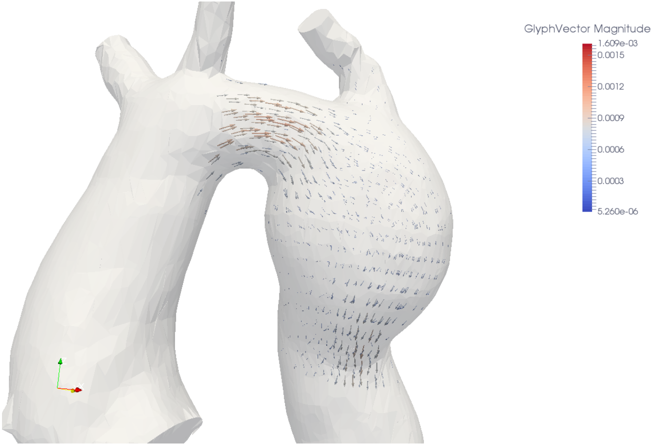
8- Koopman-mode 5

$|\lambda_5| = 0.99786 \; arg(\lambda_5) = 18.235 \approx 8 \; x \; arg(\lambda_6) \; rel.norm = 0.429$



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Performance aspects

The procedure uses the following operations

- matrix x matrix multiplication for small and large dense matrices.
- calculation of symmetric eigenproblems
- calculation of generalized symmetric eigenproblems
- roots of large polynomials in 1D to be found
- If for most of the vectors we have $v_l \approx 0$ the method can be used as problem adapted data compression method.

The matrix of measurements G might be very large (number of DOFs at all nodes for the number of time steps).

- IO is very important because of the potentially large data size
- see the talk of Erich Focht

Conclusions

- An unsteady nonlinear problem with an quasiperiodic characteristic may be approximately decomposed in a sum of complex stationary modes mulipliedby terms λ_l^k repesenting the time behaviour.
- Ensembles of trajectories with different initial states can be analysed together leading to common eigenvalues.
- The method allow for the analysis of measurements governed by hidden operators.
- The Koopman-vectors v_l have a regular behaviour. What is their physical meaning?

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Thank you for your attention

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