Computation of Contraction Metrics with Meshfree Collocation

Peter Giesl

University of Sussex, UK – Department of Mathematics
supported by the Dr Perry James (Jim) Browne Research Centre

15th December 2024
CDC Workshop on "Contraction Theory for Systems, Control, Optimization, and Learning"

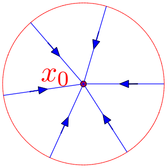
joint work with
Holger Wendland, Bayreuth, Germany
Sigurdur Hafstein, Iceland
Iman Mehrabinezhad, Cyprus

Overview

1. Contraction metric
2. Construction of contraction metric
   - Mesh-free collocation for matrix-valued functions
   - Examples
3. Verification
   - Interpolation with CPA (continuous piecewise affine) functions
   - Examples
4. Periodic orbit

System of autonomous ordinary differential equations

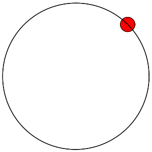
(1) $$\begin{cases} \dot{x} & = & f(x) \\ x(0) & = & \xi \end{cases}$$



$x \in \mathbb{R}^n$, $f \in C^\sigma(\mathbb{R}^n, \mathbb{R}^n)$ where $\sigma \geq 1$, $n \in \mathbb{N}$.
Flow $S_t\xi := x(t)$, solution of (1)

Equilibrium

- equilibrium x_0 $(f(x_0) = 0)$,
- basin of attraction $A(x_0) := \{\xi \in \mathbb{R}^n \mid S_t\xi \stackrel{t\to\infty}{\longrightarrow} x_0\}$



Periodic orbit

- periodic orbit $\Omega = \{S_t x \mid t \in [0, T)\}$ with $x = S_T x$
- basin of attraction $A(\Omega) = \{\xi \in \mathbb{R}^n \mid \text{dist}(S_t\xi, \Omega) \stackrel{t\to\infty}{\longrightarrow} 0\}$

Methods to determine basin of attraction

- Set oriented methods (cell mapping)
- Invariant manifolds (boundary of basin of attraction)
- Lyapunov function (distance to attractor)
- Contraction metric (distance between adjacent solutions) [Borg 1960, Hartman & Olech 1962, Krasovskii 1963, Kravchuk, Leonov & Ponomarenko 1992, Lohmiller & Slotine 1998, Forni & Sepulchre 2014, Bullo 2023]

Riemannian metric

Definition (Riemannian metric)

A matrix-valued function $M \in C^1(\mathbb{R}^n, \mathbb{S}^{n\times n})$ (symmetric $n \times n$ matrices) is called Riemannian metric if $M(x)$ is a positive definite matrix for each $x \in \mathbb{R}^n$.

Note: $\langle v, w\rangle_{M(x)} := v^T M(x) w$ defines a point-dependent scalar product for $v, w \in \mathbb{R}^n$. $M(x) = I$ gives Euclidean metric.

Definition (Orbital derivative)

For $M \in C^1(\mathbb{R}^n, \mathbb{S}^{n\times n})$, the orbital derivative is defined component-wise

$$(\dot{M}(x))_{ij} = \nabla M_{ij}(x) \cdot f(x)$$

Sufficient condition (with contraction metric)

Theorem

- $\varnothing \neq K \subset \mathbb{R}^n$ *is positively invariant, compact and connected*
- *Riemannian metric* $M \in C^1(\mathbb{R}^n, \mathbb{S}^{n\times n})$

$$Df(x)^T M(x) + M(x) Df(x) + \dot{M}(x) \prec 0 \text{ for all } x \in K$$

Then

- *Existence and uniqueness of an exponentially asymptotically stable equilibrium* $x_0 \in K$
- $K \subset A(x_0)$ *(basin of attraction)*

Converse theorem: matrix equation

Theorem (Giesl 2015/17)

Consider $\dot{x} = f(x)$, $f \in C^s(\mathbb{R}^n, \mathbb{R}^n)$, $s \geq 2$.

- x_0 *exponentially stable equilibrium*
- $C \in C^{s-1}(A(x_0), \mathbb{S}^{n\times n})$, $C(x)$ *positive definite*

Then there is a unique solution $M \in C^{s-1}(A(x_0), \mathbb{S}^{n\times n})$ *to the matrix equation*

$$Df(x)^T M(x) + M(x) Df(x) + \dot{M}(x) = -C(x) \qquad \text{for all } x \in A(x_0).$$

M *is Riemannian metric (in particular positive definite).*

Proof: $M(x) = \int_0^\infty \phi(\tau, 0; x)^T C(S_\tau x) \phi(\tau, 0; x)\, d\tau$ where $\phi(t, t_0; x)$ is the principal fundamental matrix solution of first variation equation

$$\dot{y} = Df(S_t x) y$$

2. Construction of contraction metric

Problem Find $S \in C^1(K; \mathbb{S}^{n \times n})$ such that

- $S(x) \succ 0$ (positive definite)
- $Df(x)^T S(x) + S(x) Df(x) + \dot{S}(x) \prec 0$ (negative definite)

Construction methods

- SOS (sum of squares) – Linear Matrix Inequalities (Aylward, Parrilo & Slotine 2008, polynomial systems)
- CPA (continuous piecewise affine) – semidefinite optimization (Giesl & Hafstein 2013)
- RBF (Radial Basis Functions) – mesh-free collocation (Giesl & Wendland 2018/19)

Idea

- Solution M of matrix-valued PDE $Df(x)^T M(x) + M(x) Df(x) + \dot{M}(x) = -C \prec 0$ solves problem
- Solve PDE approximately by S

2.1 Construction of contraction metric with mesh-free collocation – overview

- Linear differential operator F of order 1

$$F(M)(x) := Df(x)^T M(x) + M(x)Df(x) + \dot{M}(x)$$

- Approximate solution M of $F(M)(x) = -C \prec 0$ (matrix-valued PDE) by S
- $K \subset \mathbb{R}^n$ compact, $X = \{x_1, \ldots, x_N\} \subset K$ given collocation points
- Error estimate (from mesh-free collocation)

$$\|F(M) - F(S)\|_{L_\infty(K;\mathbb{S}^{n\times n})} \leq c_1\, h_{X,K}^{\sigma-1-n/2} \|M\|_{H^\sigma(\Omega;\mathbb{S}^{n\times n})}$$

where $h_{X,K} = \max_{y\in K} \min_{x\in X} \|x - y\|$ fill distance of collocation points

- Error estimate (from formula for M)

$$\|M - S\|_{L_\infty(K;\mathbb{S}^{n\times n})} \leq c_2 \|F(M) - F(S)\|_{L_\infty(\overline{\gamma^+(K)};\mathbb{S}^{n\times n})}$$

- This shows: $S(x)$ positive definite and $F(S)(x)$ negative definite if collocation points are dense enough

Optimal recovery

Generalised interpolation in Hilbert space H

- $\lambda_1, \dots, \lambda_M \in H^*$ linearly independent functionals
- $r_1, \dots, r_M \in \mathbb{R}$ given

Optimal recovery: $S \in H$ such that

$$\|S\|_H = \min\{\|S\|_H, \lambda_i(S) = r_i \text{ for } i = 1, \dots, M\}$$

- Solution $S = \sum_{j=1}^M \beta_j v_j$, v_j Riesz representer of λ_j, $\beta_j \in \mathbb{R}$
- Interpolation condition $\lambda_i(S) = \sum_{j=1}^M \beta_j \lambda_i(v_j) = r_i$ for $i = 1, \dots, M$: system of linear equations

Optimal recovery of matrix-valued functions

Generalised interpolation in Hilbert space $H= H^\sigma(\Omega; \mathbb{S}^{n\times n})$, which is a Reproducing Kernel Hilbert Space: special form of Riesz representer

Functionals

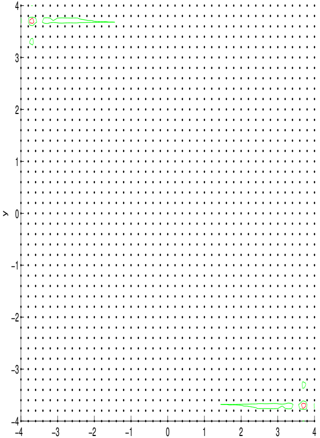
- $F\colon H^\sigma(\Omega; \mathbb{S}^{n\times n}) \to H^{\sigma-1}(\Omega; \mathbb{S}^{n\times n})$ differential operator of order 1: $F(M) = Df(x)^T M(x) + M(x)Df(x) + \dot{M}(x)$
- $X = \{x_1, \ldots, x_N\} \subset \Omega$ collocation points
- $\lambda_k^{(i,j)}(M) = e_i^T F(M)(x_k)e_j$, $1 \leq i \leq j \leq n$, $k = 1, \ldots, N$ linearly independent functionals
- solve system of linear equations of size $N\frac{n(n+1)}{2}$

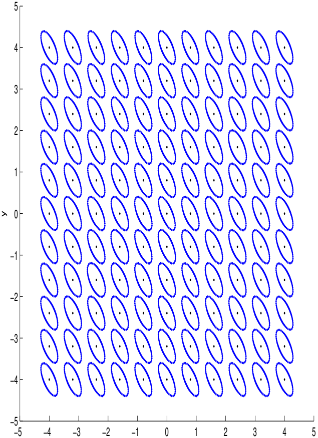
Linear example

$$\begin{aligned} \dot{x} &= -x + y \\ \dot{y} &= x - 2y \end{aligned}$$

- $X = \{(x, y) \in \mathbb{R}^2 \mid x, y = -4, -3.8, -3.6, \ldots, 0, 0.2, \ldots, 4\}$ with $N = 1681$ points
- linear system with 5043×5043 matrix
- Solution of $F(M)(x) = -I$ is $M(x) = \begin{pmatrix} 1 & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix}$

Linear example

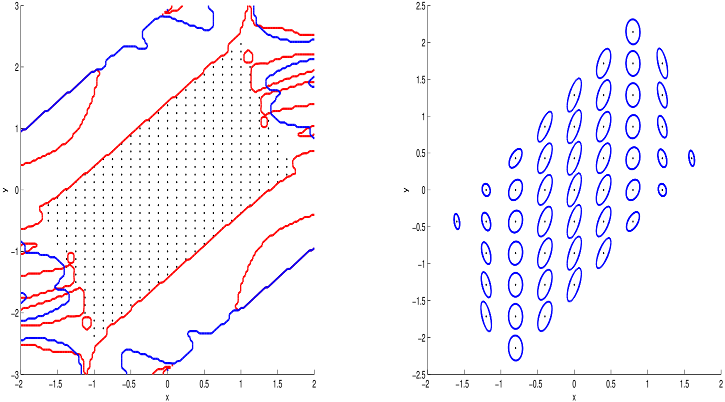




Left: Collocation points; $\operatorname{tr} F(S)(x,y) = 0$ (red) and $\det F(S)(x,y) = 0$ (green).

Right: Curve of equal distance with respect to metric $S(x)$:
$\{x + v \mid (v - x)^T S(x)(v - x) = \text{const}\}$

Van der Pol with reversed time $\begin{aligned} \dot{x} &= -y \\ \dot{y} &= x - 3(1-x^2)y \end{aligned}$

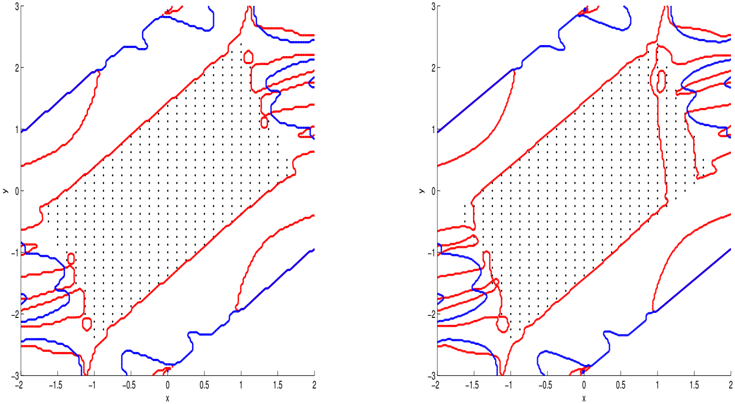


Left: Collocation points; $F(S)(x,y) \prec 0$ (red) and $S(x,y) \succ 0$ (blue)
Right: Curve of equal distance with respect to metric $S(x,y)$

Perturbed van der Pol

$$\begin{aligned}\dot{x} &= -y + \epsilon \\ \dot{y} &= x - (3+\epsilon)(1-x^2)y\end{aligned}$$

$\epsilon = 0.1$



Left: Collocation points; $F(S)(x,y) \prec 0$ (red) and $S(x,y) \succ 0$ (blue)
Right: Collocation points; $F_\epsilon(S)(x,y) \prec 0$ (red) and $S(x,y) \succ 0$ (blue)

3. Verification

Problem: how to verify $F(S)(x) \prec 0$ and $S(x) \succ 0$?

- Error estimates do not provide explicit bound
- and hold only in the (unknown) basin of attraction

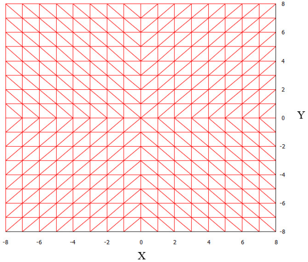
Idea:

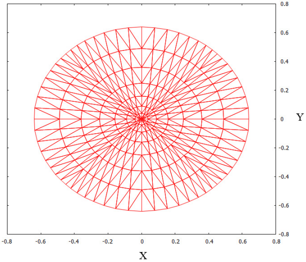
- interpolate metric by continuous piecewise affine (CPA) metric on triangulation
- Taylor-type estimates at vertices ensure rigorous verification of conditions

Triangulation

- Simplicial complex (triangulation) is a collection $\mathcal{T}$ of simplices $\mathcal{S} = \mathrm{co}(x_0, x_1, \ldots, x_n)$
- Vertex set $\mathcal{V}_{\mathcal{T}}$, e.g. $\rho\mathbb{Z}^n$
- Largest distance of vertices in a simplex h_ν

Examples of triangulations





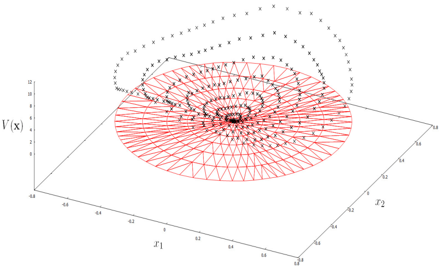
CPA interpolation of (matrix-valued) function

CPA interpolation P of S:

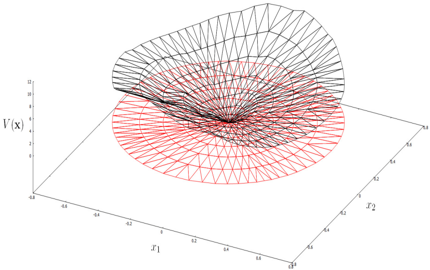
i) $P(x) := S(x)$ for every vertex $x \in \mathcal{V}_{\mathcal{T}}$

ii) P_{ij} is affine on every simplex $\mathcal{S}_\nu \in \mathcal{T}$

Values at vertices



CPA interpolation



CPA estimates: constraints

1. **Positive definiteness of $\mathbf{P}$**: $P(x_k) \succeq \epsilon_0 I \qquad \forall x_k \in \mathcal{V}_\mathcal{T}$
2. **Upper bound on $\mathbf{P}$**: $P(x_k) \preceq C_\nu I \qquad \forall x_k \in \mathcal{V}_\mathcal{T}$
3. **Bound on the derivative of $\mathbf{P}$**: $\forall \mathcal{S}_\nu \in \mathcal{T}, i,j \in \{1,\ldots,n\}$
   $\left\| \nabla P_{ij}\big|_{\mathcal{S}_\nu^\circ} \right\|_1 \le D_\nu$
4. **Negative definiteness of contraction condition**: for each simplex $\mathcal{S}_\nu = \mathrm{co}(x_0,\ldots,x_n) \in \mathcal{T}$, $\forall$ vertex x_k of $\mathcal{S}_\nu$:

$$\begin{aligned} -\epsilon_0 I \;\succeq\; & P(x_k)Df(x_k) + Df(x_k)^T P(x_k) \\ & + (\nabla P_{ij}\big|_{\mathcal{S}_\nu^\circ} \cdot f(x_k))_{i,j=1,2,\ldots,n} + h_\nu^2 E_\nu I \end{aligned}$$

$E_\nu := n^2(1+4\sqrt{n})B_{2,\nu}D_\nu + 2\,n^3 B_{3,\nu}C_\nu$
($B_{\cdot,\nu}$: bounds on 2nd and 3rd derivatives of f)

Theorem

If constraints are satisfied, then P is contraction metric.

Converse result

$$M \quad \overset{\text{collocation points}}{\underset{\text{RBF approximation}}{\longrightarrow}} \quad S \quad \overset{\text{triangulation}}{\underset{\text{CPA interpolation}}{\longrightarrow}} \quad P$$

Theorem

If

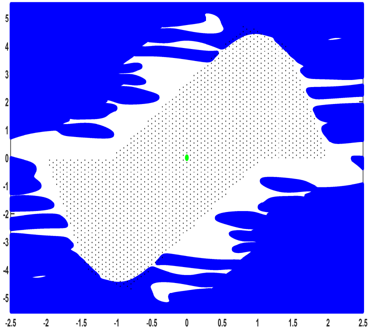
- *collocation points sufficiently dense and*
- *triangulation sufficiently fine*

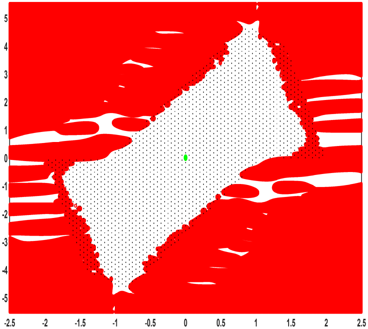
then

- *CPA interpolation* P *of*
- *RBF approximation* S *of*
- *the solution* M *of PDE*

satisfies the constraints.

3.2 Examples: Van der Pol $\begin{aligned}\dot{x} &= -y \\ \dot{y} &= x - 3(1-x^2)y\end{aligned}$

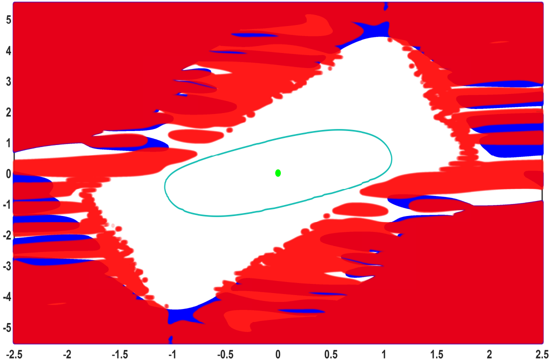




Black: 1926 collocation points
Blue: $P(x)$ not positive definite

Green: equilibrium
Red: *Constraint 4* not satisfied

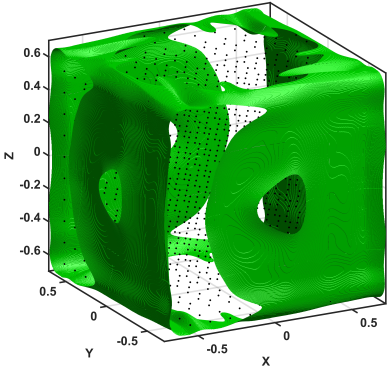
Example: Van der Pol $\begin{aligned} \dot{x} &= -y \\ \dot{y} &= x - 3(1-x^2)y \end{aligned}$

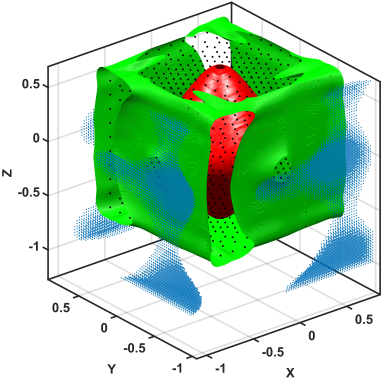


Dark green: positively invariant set (using Lyapunov-like function)

3-d example:

$$\begin{aligned} \dot{x} &= x(x^2+y^2-1) - y(z^2+1) \\ \dot{y} &= y(x^2+y^2-1) + x(z^2+1) \\ \dot{z} &= 10z(z^2-1) \end{aligned}$$





Green: *Constraint 4* not satisfied

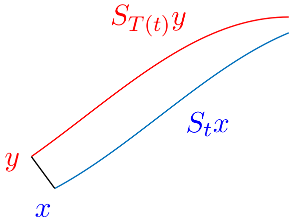
Red: positively invariant set

4. Contraction criterion for periodic orbit

Differences to equilibrium

- No contraction in direction of flow
- Orbital stability requires synchronisation of time of solutions such that difference vector perpendicular to f

$$(S_{T(t)}y - S_t x)^T f(S_t x) \;\; = \;\; 0$$



Sufficient condition (with Riemannian metric)

Theorem (Giesl 2021)

- $\varnothing \neq K \subset \mathbb{R}^n$ *positively invariant, compact, connected, no equilibrium*
- *Riemannian metric* $M \in C^1(\mathbb{R}^n, \mathbb{S}^{n\times n})$
- $P_x := I - \frac{f(x)f(x)^T}{\|f(x)\|^2}$ *projection onto hyperplane* $\perp f(x)(\neq 0)$

$$\begin{aligned} LM(x) &:= Df(x)^T M(x) + M(x)Df(x) + \dot{M}(x) \\ &\quad - \frac{M(x)f(x)f(x)^T(Df(x)+Df(x)^T)}{\|f(x)\|^2} \\ &\quad - \frac{(Df(x)+Df(x)^T)f(x)f(x)^T M(x)}{\|f(x)\|^2} \\ LM(x) &= -P_x^T B(x) P_x \\ \text{with } B(x) &\succ 0 \end{aligned}$$

Then: existence and uniqueness of exponentially asymptotically stable periodic orbit $\Omega \subset K$ *and* $K \subset A(\Omega)$ *(basin of attraction)*

Converse theorem: matrix equation

Theorem (Giesl 2021)

Consider $\dot{x} = f(x)$, $f \in C^\sigma(\mathbb{R}^n, \mathbb{R}^n)$, $\sigma \geq 2$.

- Ω *exponentially stable periodic orbit*
- $B \in C^{\sigma-1}(A(\Omega), \mathbb{S}^{n\times n})$, $B(x) \succ 0$
- $\xi_0 \in A(\Omega)$, $c_0 > 0$

Then there is a unique solution $M \in C^{\sigma-1}(A(\Omega), \mathbb{S}^{n\times n})$ *to*

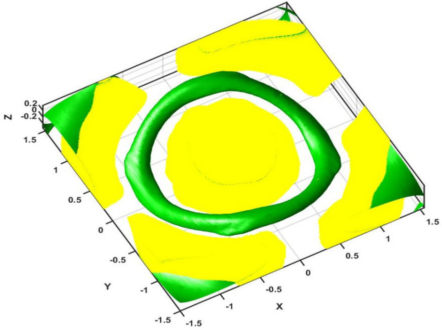
$$\begin{aligned} LM(x) &= -P_x^T B(x) P_x =: -C(x) \text{ for all } x \in A(\Omega) \\ \text{with } f(\xi_0)^T M(\xi_0) f(\xi_0) &= c_0 \|f(\xi_0)\|^4 \end{aligned}$$

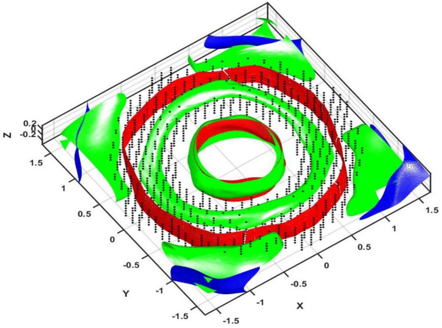
M *is Riemannian metric (in particular positive definite).*

Proof: $M(x) = \int_0^\infty \phi(\tau, 0; x)^T C(S_\tau x) \phi(\tau, 0; x)\, d\tau + c_0 f(x) f(x)^T$ where $\phi(t, t_0; x)$ is principal fundamental matrix solution of first variation equation $\dot{y} = Df(S_t x) y$

Example

$$\begin{aligned}\dot{x} &= x(1-x^2-y^2)-y+0.1yz\\ \dot{y} &= y(1-x^2+y^2)+x\\ \dot{z} &= -z+xy\end{aligned}$$





Black: 3256 collocation points
Blue: S not positive definite

Green: positively invariant set
Red: LS not negative definite

Summary

- Contraction metric (local property, distance between adjacent trajectories)
- Determination of equilibrium/periodic orbit and its basin of attraction
- No information about attractor needed
- Robust with respect to perturbations
- Converse theorems, characterised by linear matrix-valued PDE
- Numerical construction by solving matrix-valued PDE with mesh-free collocation
- Verification by interpolating with CPA metric and checking inequalities

Some references

- P. Giesl, *Converse theorems on contraction metrics for an equilibrium*, *J. Math. Anal. Appl.* 424 (2015), 1380–1403.
- P. Giesl & H. Wendland, *Kernel-based Discretisation for Solving Matrix-Valued PDEs*. *SIAM J. Numer. Anal.*, **56** (2018), 3386–3406.
- P. Giesl & H. Wendland, *Construction of a Contraction Metric by Meshless Collocation*. *Discrete Contin. Dyn. Syst. Ser. B* **24** (2019), 3843–3863.
- P. Giesl, *Computation of a contraction metric for a periodic orbit*. *SIAM J. Appl. Dyn. Syst.* **18** (2019), 1536–1564.
- P. Giesl, *On a matrix-valued PDE characterizing a contraction metric for a periodic orbit*. *Discrete Contin. Dyn. Syst. Ser. B* **20** (2021), 4839–4865.
- P. Giesl, S. Hafstein & I. Mehrabinezhad, *Computation and verification of contraction metrics for equilibria*. *J. Comp. Appl. Math.* **390** (2021), Article 113332.
- P. Giesl, S. Hafstein & I. Mehrabinezhad, *Computation and verification of contraction metrics for periodic orbits*. *J. Math. Anal. Appl.* **503** (2021), Article 125309.
- P. Giesl, S. Hafstein & C. Kawan, *Review on contraction analysis and computation of contraction metrics*, *J. Comp. Dyn.*, **10** (2023), 1–47