Community integration algorithms (CIAs): A novel computational approach for large-scale dynamical systems and extensions to networks

Mechthild Thalhammer
Leopold–Franzens-Universität Innsbruck, Austria

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References

Former contributions.

T. Böhle, Ch. Kühn, M. Th.

On the reliable and efficient numerical integration of the Kuramoto model and related dynamical systems on graphs. International Journal of Computer Mathematics (2021).

Dedicated to Jesús María Sanz-Serna due to his seminal contributions in the area of geometric numerical integration.

Community integration algorithms (CIAs) for dynamical systems on networks. Journal of Computational Physics 469 (2022).

Current and related investigations.

J. A. Carrillo, M. Th.

Novel approaches for the reliable and efficient numerical evaluation of the Landau operator. Communications in Computational Physics (2026).

On the efficient time integration of the deterministic particle system associated with the Stein variational gradient descent method.

Guide line

Large-scale classical dynamical systems.

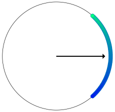
- Algorithms for the evaluation of the defining functions
- Issues and novel approaches

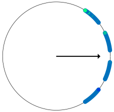
Extended systems on networks / graphs.

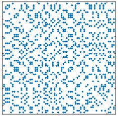
- Algorithms for the detection of communities
- Suitable modifications of novel approaches

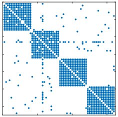
Widely-used models with relevant applications.

- Classical and extended Kuramoto systems
- Synchronisation of coupled oscillators



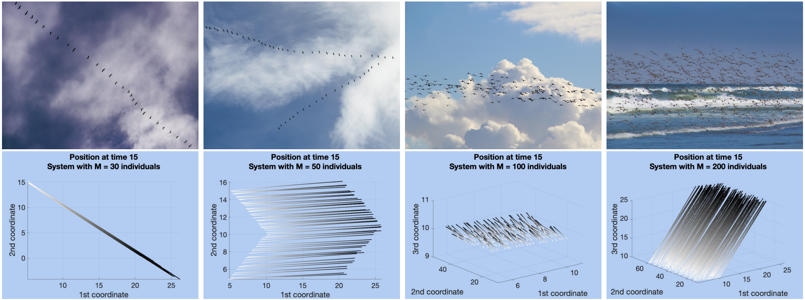






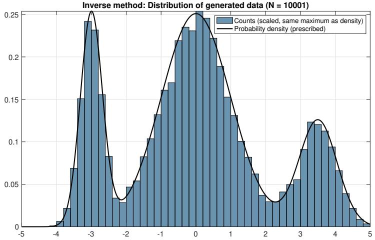
Further areas of application

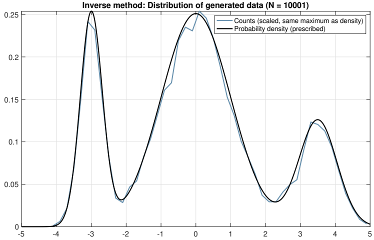
Cucker–Smale flocking models. Employ additional Fourier series representations of defining functions.



Further areas of application

Generation of samples for probability distributions. Provide alternative approaches that are suitable for high(er)-dimensional problems based on long-term integrations of deterministic particle systems.





Multi-particle systems

Study of Kuramoto systems as starting point of our works.
Classical systems correspond to the special cases of complete graphs.

Basic ingredients

Basic ingredients.

- Consider dynamical multi-particle systems of the form

$$\begin{cases} y'(t) = F\big(y(t)\big), & t \in (0,T), \\ y(0) \text{ given}. \end{cases}$$

- Algorithms for the reliable and efficient evaluation of the defining functions (for fixed $t \in [0,T]$) constitute basic ingredients regarding numerical simulations (e.g. time integration, optimisation).

Kuramoto systems

Kuramoto systems.

- Consider a set of oscillators with time-dependent phases

$$\vartheta_m : [0,T] \longrightarrow \mathbb{S}_1 = \mathbb{R}/2\pi\mathbb{Z}, \quad m \in \{1,2,\dots,M\}.$$

- Prescribe the intrinsic frequencies and the coupling constant

$$\omega_m \in \mathbb{R}, \quad m \in \{1,2,\dots,M\}, \quad K > 0.$$

- Describe the pairwise interactions between the oscillators by a system of coupled nonlinear ordinary differential equations

$$\begin{cases} \vartheta_m'(t) = \omega_m + \frac{K}{M} \sum_{\ell=1}^{M} \sin\big(\vartheta_\ell(t) - \vartheta_m(t)\big), & t \in (0,T), \\ \vartheta_m(0) \text{ given}, & m \in \{1,2,\dots,M\}. \end{cases}$$

Kuramoto systems

Large-scale systems.

- Focus on systems involving a high number of oscillators

$$M \gg 1 \,.$$

Special choices.

- Consider uniformly distributed initial phases (average arises in conserved quantity)

$$\vartheta_m(0) = \tfrac{2\pi m}{M}\,, \quad m \in \{1,2,\dots,M\}\,, \quad \tfrac{1}{M} \sum_{m=1}^{M} \vartheta_m(0) = \big(1 + \tfrac{1}{M}\big)\,\pi\,.$$

- Define the intrinsic frequencies by (average arises in conserved quantity)

$$\omega_m = 1 + \omega_0\,\tfrac{(2m-M-1)}{M-1} \in [1-\omega_0, 1+\omega_0]\,, \quad \omega_0 \geq 0\,, \quad m \in \{1,2,\dots,M\}\,,$$
$$\tfrac{1}{M} \sum_{m=1}^{M} \omega_m = 1\,.$$

Quadratic complexity

Computational complexity.

- For Kuramoto systems, the naive evaluation of the decisive sums

$$\sum_{\ell=1}^{M} \sin\big(\vartheta_\ell(t) - \vartheta_m(t)\big), \quad m \in \{1, 2, \dots, M\},$$

requires in total M^2 sine function evaluations.

- Same conclusions for other multi-particle systems such as Cucker–Smale models and the sampling problem.
- Quadratic computational complexity considerably reduces practicability. Typically, we reach a critical range for

$$M = 10^5, \quad M^2 = 10^{10}.$$

Quadratic complexity

Quadratic complexity.

- It is highly desirable to avoid quadratic complexity, since it effects the allocatable memory capacity and the computation time.
- For standard programming and numeric computing platforms, we are confronted with a severe restriction of the maximum dimension.

Is a reduction from quadratic to linear complexity feasible?

Error message in MATLAB.

Requested 10000000000x1 (74.5GB) array exceeds maximum array size preference. Creation of arrays greater than this limit may take a long time and cause MATLAB *to become unresponsive.*

Out of memory for a vector of dimension 10^{10}.
Out of memory for a matrix of dimension 10^5.

Quadratic complexity

Natural idea.

- Use a compact matrix representation and sum over all columns

$$\begin{pmatrix} s_{11}(t) & s_{12}(t) & \dots & \dots & s_{1M}(t) \\ s_{21}(t) & s_{22}(t) & \dots & \dots & s_{2M}(t) \\ \vdots & & & & \vdots \\ s_{M1}(t) & s_{M2}(t) & \dots & s_{M,M-1}(t) & s_{MM}(t) \end{pmatrix},$$

$$s_{\ell m}(t) = \sin\big(\vartheta_\ell(t) - \vartheta_m(t)\big), \quad \ell, m \in \{1, 2, \dots, M\},$$

$$\sum_{\ell=1}^{M} \sin\big(\vartheta_\ell(t) - \vartheta_m(t)\big) = \sum_{\ell=1}^{M} s_{\ell m}(t), \quad m \in \{1, 2, \dots, M\}.$$

This representation is convenient, but quadratic complexity remains!

MATLAB script by Cleve Moler.
% theta-theta' is a matrix with elements theta(j)-theta(k).
% The sum is by colums and produces a column vector.
g = sum(sin(theta-theta'),2);
See https://blogs.mathworks.com/cleve/2019/10/30/stability-of-kuramoto-oscillators.

Quadratic complexity

Natural idea – modification.

- Omit zero entries and use anti-symmetry of sine function

$$s_{\ell m}(t) = \sin\big(\vartheta_\ell(t) - \vartheta_m(t)\big) = -\, s_{m\ell}(t)\,, \quad \ell, m \in \{1,2,\dots,M\}\,,$$

$$\begin{pmatrix} 0 & s_{12}(t) & \dots & \dots & s_{1M}(t) \\ -\,s_{12}(t) & 0 & s_{23}(t) & \dots & s_{2M}(t) \\ \vdots & & & & \vdots \\ -\,s_{1M}(t) & \dots & \dots & -\,s_{M-1,M}(t) & 0 \end{pmatrix}.$$

- Number of sine function evaluations

$$(M-1) + (M-2) + \cdots + 2 + 1 \underset{\text{Kleiner Gauß}}{=} \tfrac{1}{2}\, M\,(M-1) = \mathcal{O}\big(M^2\big)\,.$$

This representation is useful to recognise a conserved quantity, but quadratic complexity still remains!

Linear complexity

Novel approach.

- Based on the addition theorem for the sine function

$$\sin\big(\vartheta_\ell(t)-\vartheta_m(t)\big)=\sin\big(\vartheta_\ell(t)\big)\cos\big(\vartheta_m(t)\big)-\cos\big(\vartheta_\ell(t)\big)\sin\big(\vartheta_m(t)\big)$$

and the precomputation of sums

$$S_M\big(\vartheta(t)\big)=\sum_{m=1}^{M}\sin\big(\vartheta_m(t)\big)\,,\quad C_M\big(\vartheta(t)\big)=\sum_{m=1}^{M}\cos\big(\vartheta_m(t)\big)\,,$$

we obtain a suitable reformulation that permits the simultaneous evaluation of the right-hand side and requires $4M$ evaluations of sine and cosine functions $(m\in\{1,2,\dots,M\})$

$$\sum_{\ell=1}^{M}\sin\big(\vartheta_\ell(t)-\vartheta_m(t)\big)=S_M\big(\vartheta(t)\big)\cos\big(\vartheta_m(t)\big)-C_M\big(\vartheta(t)\big)\sin\big(\vartheta_m(t)\big)\,.$$

Extensions

Underlying structure.

- Representations of defining functions by trigonometric polynomials
- Multiplicativity of complex exponentials permits separation of dependencies on particles

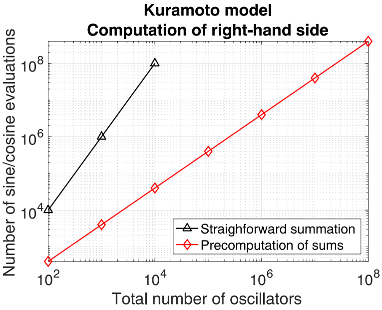
Extensions.

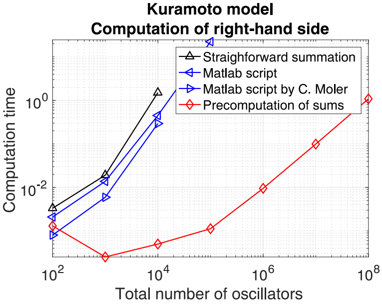
- Approximations by truncated Fourier series

Illustration (Complexity)

Computational cost for the evaluation of the function defining the right-hand side of the classical Kuramoto model.

- Number of sine and cosine evaluations versus the total number of oscillators when using straighforward summation and the precomputation of sums, respectively.
- Numerical comparison of the computation time for different implementations in MATLAB.





Structural properties of Kuramoto systems
Numerical illustrations

Structural properties

Potential.

- Kuramoto systems have the intrinsic structure of gradient systems

$$\begin{cases} \vartheta'(t) = -\nabla V\big(\vartheta(t)\big), \quad t \in (0,T), \\ \vartheta(0) \text{ given}. \end{cases}$$

- A compact representation of the associated potential reads as

$$V : \mathbb{R}^M \longrightarrow \mathbb{R} :$$
$$\vartheta = (\vartheta_1, \dots, \vartheta_M)^T \longmapsto -\omega^T \vartheta + \tfrac{KM}{2} \Big(1 - \big(C_M(\vartheta)\big)^2 - \big(S_M(\vartheta)\big)^2\Big).$$

- A short calculation confirms that the values of the potential indeed decrease when time evolves

$$\tfrac{\mathrm{d}}{\mathrm{d}t} V\big(\vartheta(t)\big) = \Big(\nabla V\big(\vartheta(t)\big)\Big)^T \vartheta'(t) = -\big\|\nabla V\big(\vartheta(t)\big)\big\|^2 \leq 0,$$
$$V\big(\vartheta(t)\big) \leq V\big(\vartheta(0)\big), \quad t \in [0,T].$$

Structural properties

Conserved quantity.

- From the representation (with $s_{\ell m} = \sin(\vartheta_\ell - \vartheta_m)$)

$$\begin{cases} \vartheta'_m(t) = \omega_m + \frac{K}{M} \sum_{\ell=1}^{M} s_{\ell m}(t) \,, \quad t \in (0,T) \,, \\ \vartheta_m(0) \text{ given} \,, \quad m \in \{1,2,\dots,M\} \,, \end{cases}$$

$$\begin{pmatrix} 0 & s_{12}(t) & \dots & \dots & s_{1M}(t) \\ -s_{12}(t) & 0 & s_{23}(t) & \dots & s_{2M}(t) \\ \vdots & & & & \vdots \\ -s_{1M}(t) & \dots & \dots & -s_{M-1,M}(t) & 0 \end{pmatrix}, \quad t \in (0,T) \,,$$

it is evident that summation over all governing equations (i.e. all entries of the associated matrix) and integration with respect to time yields

$$\frac{1}{M} \sum_{m=1}^{M} \vartheta'_m(t) = \frac{1}{M} \sum_{m=1}^{M} \omega_m \,, \quad \frac{1}{M} \sum_{m=1}^{M} \vartheta_m(t) = \frac{1}{M} \sum_{m=1}^{M} \vartheta_m(0) + t\, \frac{1}{M} \sum_{m=1}^{M} \omega_m \,, \quad t \in [0,T] \,.$$

- Thus, the mean values of the initial phases and the intrinsic frequencies determine the mean values of the phases at later times.

Synchronisation through coupling

Mechanisms.

- The independent motion of an oscillator is determined by its intrinsic frequency.
- The coupling term enhances synchronisation of oscillators (for $\vartheta_\ell \approx \vartheta_m$), since it accelerates slower oscillators ($\sin(\vartheta_\ell - \vartheta_m) > 0$ when $\vartheta_\ell > \vartheta_m$) and decelerates faster oscillators ($\sin(\vartheta_\ell - \vartheta_m) < 0$ when $\vartheta_\ell < \vartheta_m$).

Order parameter.

- The modulus $r : \mathbb{S}_1^M \to \mathbb{R}$ and the angle $\psi : \mathbb{S}_1^M \to \mathbb{R}$ of the complex order parameter are given by

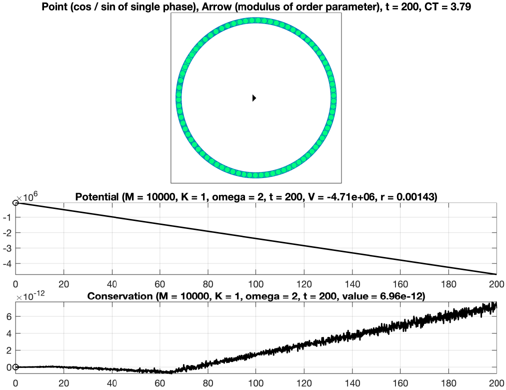
$$r(\vartheta)\, \mathrm{e}^{\mathrm{i}\,\psi(\vartheta)} = \frac{1}{M} \sum_{m=1}^{M} \mathrm{e}^{\mathrm{i}\,\vartheta_m} = C_M(\vartheta) + \mathrm{i}\, S_M(\vartheta)\,, \quad \vartheta \in \mathbb{S}_1^M\,.$$

- For configurations, where all cosine and sine values are close-by, the modulus of the complex order parameter has values nearly one and thus indicates synchronisation

$$\cos(\vartheta_m) \approx \cos(\vartheta_1)\,, \quad \sin(\vartheta_m) \approx \sin(\vartheta_1)\,, \quad m \in \{2, 3, \dots, M\}\,,$$
$$C_M(\vartheta) \approx \cos(\vartheta_1)\,, \quad S_M(\vartheta) \approx \sin(\vartheta_1)\,,$$
$$r(\vartheta) = \sqrt{\big(C_M(\vartheta)\big)^2 + \big(S_M(\vartheta)\big)^2} \approx 1\,, \quad V(\vartheta) \approx -\omega^T \vartheta\,, \quad \vartheta \in \mathbb{S}_1^M\,.$$

Numerical illustrations (No synchronisation)

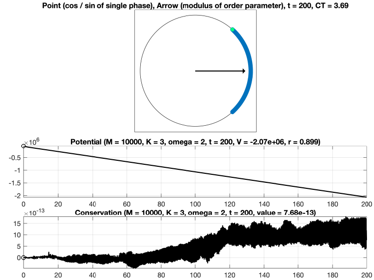
Numerical integration of the classical Kuramoto model involving $M = 10^4$ oscillators. The time series confirms decreasing potential values and preservation of a conserved quantity with high accuracy. Visualisation of a phase at the final time by a point on the unit circle $\cos(\vartheta_m) + \sin(\vartheta_m)$. For smaller values of the coupling constant ($K = 1$), no synchronisation is observed (modulus of order parameter close to one).

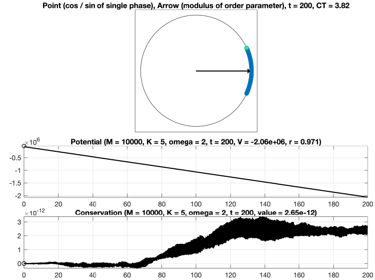


http://techmath.uibk.ac.at/mecht/MyHomepage/Research/MovieKuramotoClassicalK1.m4v

Numerical illustrations (Gradual synchronisation)

Numerical integration of the classical Kuramoto model involving $M = 10^4$ oscillators. For larger values of the coupling constant ($K \in \{3, 5\}$), gradual synchronisation is observed (order parameter close to zero).





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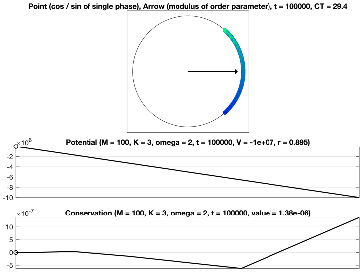
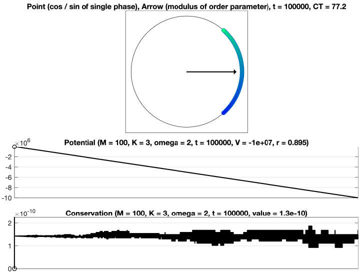
http://techmath.uibk.ac.at/mecht/MyHomepage/Research/MovieKuramotoClassicalK5.m4v

Numerical illustrations (Long-term integration)

Long-term integration of the classical Kuramoto model based on a second-order explicit Runge–Kutta method and the second-order implicit midpoint rule with improved numerical preservation of a conserved quantity (symplectic scheme).





Higher-order Kuramoto-type systems

Higher-order Kuramoto-type systems

Higher-order contributions.

- Single sums describe pairwise interactions between oscillators

$$\frac{1}{M}\sum_{\ell=1}^{M}\sin\big(\vartheta_\ell(t)-\vartheta_m(t)\big), \quad m\in\{1,2,\dots,M\}.$$

- Multiple sums describe interactions between several oscillators

$$\frac{1}{M^L}\sum_{\ell_1,\dots,\ell_L=1}^{M}\sin\big(\sigma_1\vartheta_{\ell_1}(t)+\dots+\sigma_L\vartheta_{\ell_L}(t)-\vartheta_m(t)\big),$$
$$\sigma_1,\dots,\sigma_L\in\{-1,1\}, \quad m\in\{1,\dots,M\}.$$

Poynomial complexity

Computational complexity.

- The naive evaluation of single sums

$$\sum_{\ell=1}^{M} \sin\big(\vartheta_\ell(t) - \vartheta_m(t)\big), \quad m \in \{1,2,\ldots,M\},$$

requires $\mathcal{O}(M^2)$ sine function evaluations.

- The naive evaluation of multiple sums

$$\frac{1}{M^L} \sum_{\ell_1,\ldots,\ell_L=1}^{M} \sin\big(\sigma_1 \vartheta_{\ell_1}(t) + \cdots + \sigma_L \vartheta_{\ell_L}(t) - \vartheta_m(t)\big),$$
$$\sigma_1,\ldots,\sigma_L \in \{-1,1\}, \quad m \in \{1,\ldots,M\}.$$

requires $\mathcal{O}(M^{L+1})$ sine function evaluations.

Is a reduction from polynomial to linear complexity feasible? YES!

Linear complexity

Novel approach.

- Based on the addition theorem for the sine function and the precomputation of sums

$$S_M\big(\vartheta(t)\big) = \sum_{m=1}^{M} \sin\big(\vartheta_m(t)\big)\,, \quad C_M\big(\vartheta(t)\big) = \sum_{m=1}^{M} \cos\big(\vartheta_m(t)\big)\,,$$

we obtain a suitable reformulation that permits the simultaneous evaluation of the right-hand side and requires $\mathcal{O}(M)$ evaluations of sine and cosine functions.

Example ($L = 3$). With $S_M = S_M(\vartheta)$ and $C_M = C_M(\vartheta)$, the multiple sums rewrite as

$$\begin{aligned}
&\sum_{\ell_1,\ell_2,\ell_3=1}^{M} \sin(\sigma_1\,\vartheta_{\ell_1} + \sigma_2\,\vartheta_{\ell_2} + \sigma_3\,\vartheta_{\ell_3} - \vartheta_m) \\
&\quad = \Big((\sigma_1+\sigma_2+\sigma_3)\,C_M^2 - \sigma_1\,\sigma_2\,\sigma_3\,S_M^2\Big)\,S_M \cos(\vartheta_m) \\
&\qquad + \Big((\sigma_1\,\sigma_2 + \sigma_1\,\sigma_3 + \sigma_2\,\sigma_3)\,S_M^2 - C_M^2\Big)\,C_M \sin\big(\vartheta_m(t)\big)\,, \quad m \in \{1,\dots,M\}\,.
\end{aligned}$$

Summary

Computational complexity. It is reasonable to measure the cost for the evaluation of the defining functions of classical Kuramoto systems and generalisations involving terms of order L by the number of sine and cosine function evaluations in dependence of the total number of oscillators.

- A naive formulation results in polynomial complexity.
- Suitable reformulations and precomputations of sums permit the reduction to linear complexity.

	Naive approach	Novel approach
Classical Kuramoto systems	$\mathcal{O}(M^2)$	$\mathcal{O}(M)$
Higher-order generalisations	$\mathcal{O}(M^{L+1})$	$\mathcal{O}(M)$

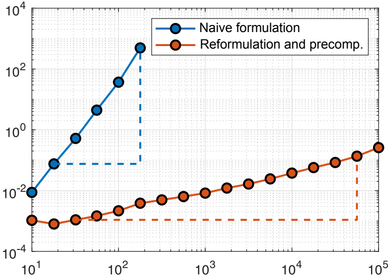
Numerical illustration

Numerical integration of a higher-order Kuramoto-type system involving a term of the form

$$\sum_{\ell_1,\ell_2,\ell_3=1}^{M} \sin(\vartheta_{\ell_1} - \vartheta_{\ell_2} + \vartheta_{\ell_3} - \vartheta_m) = \left(C_M^2 + S_M^2\right)\left(S_M \cos(\vartheta_m) - C_M \sin\left(\vartheta_m(t)\right)\right), \quad m \in \{1,\dots,M\}.$$

Computation times in seconds versus the dimensions of the system.

- A naive formulation and implementation leads to quartic complexity $\mathcal{O}(M^4)$.
- A suitable reformulation and the precomputation of sums permit the reduction to linear complexity $\mathcal{O}(M)$.



Kuramoto systems on graphs

A picture says more than a thousand words ...
... rigorous formulas are found in our papers.

Kuramoto systems on graphs

Kuramoto systems on graphs.

- Take into account pairwise interactions between certain oscillators.
- Build up the associated adjacency matrix

$$A = \big(A_{m\ell}\big)_{\ell,m\in\{1,\dots,M\}}\,,$$

$$\begin{cases} \text{Interaction between oscillators } \ell \text{ and } m: & A_{m\ell} = 1\,, \\ \text{No interaction between oscillators } \ell \text{ and } m: & A_{m\ell} = 0\,, \end{cases}$$

$$\ell, m \in \{1, 2, \dots, M\}\,.$$

Kuramoto systems on graphs

Kuramoto systems on graphs.

- The resulting system of coupled nonlinear ordinary differential equations has the form

$$\begin{cases} \vartheta_m'(t) = \omega_m + \frac{K}{\mathcal{M}_m} \sum_{\ell=1}^{M} A_{m\ell} \sin\big(\vartheta_\ell(t) - \vartheta_m(t)\big), \quad t \in (0,T), \\ \vartheta_m(0) \text{ given}, \quad m \in \{1,2,\dots,M\}. \end{cases}$$

- Common uniform scaling

$$\mathcal{M}_m = M, \quad m \in \{1,2,\dots,M\}.$$

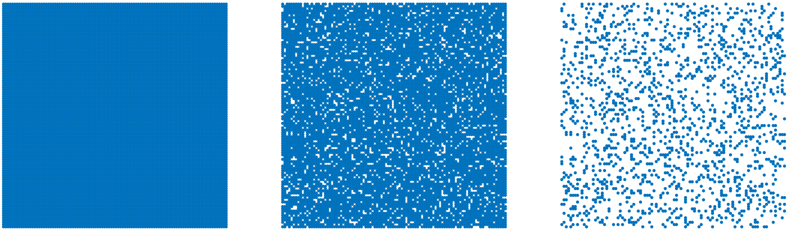
- Alternative non-uniform scaling

$$\mathcal{M}_m = \sum_{\ell=1}^{M} A_{m\ell}, \quad m \in \{1,2,\dots,M\}.$$

Kuramoto systems on graphs

Kuramoto systems on graphs.

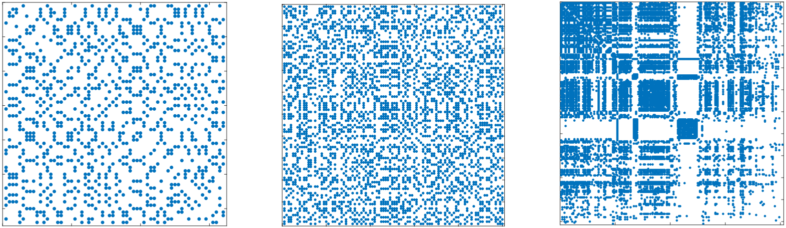
- A full matrix corresponds to a classical system (all-to-all coupling).
- A relatively dense matrix reflects relatively many interactions between the oscillators.
- A relatively sparse matrix reflects relatively few interactions between the oscillators.



Kuramoto systems on graphs

Realistic situations.

- Randomly generated adjacency matrices studied in the context of Kuramoto systems on graphs.
- Adjacency matrix associated with a real data graph for animal networks studied in the context of Cucker–Smale systems.



See https://networkrepository.com/aves-wildbird-network.php.

Computational complexity

Computational complexity.

- The number of non-zero coefficients determines the computational complexity (required memory capacity, computation time).

Natural questions.

- Is there an alternative approach to the straightforward summation of contributions corresponding to non-zero coefficients?

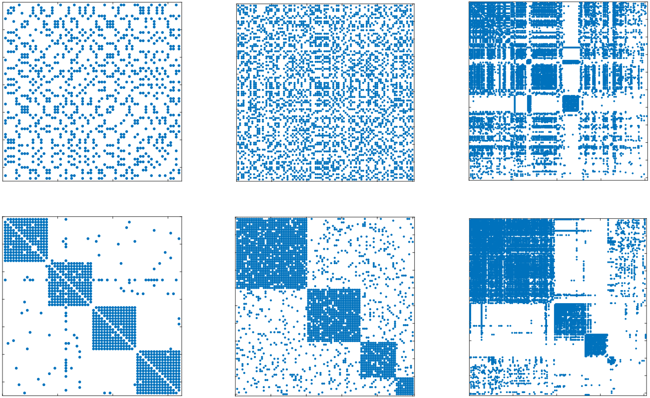
$$\sum_{\substack{\ell=1 \\ A_{m\ell}\neq 0}}^{M} \sin\big(\vartheta_\ell(t) - \vartheta_m(t)\big)\,, \quad m \in \{1,2,\dots,M\}\,.$$

- Is there a possibility to use the underlying structure of the graph?

Key idea (Pre-simulation step)

Community detection.

- Transform the underlying adjacency matrix (first row) by a permutation matrix to a block matrix (second row).



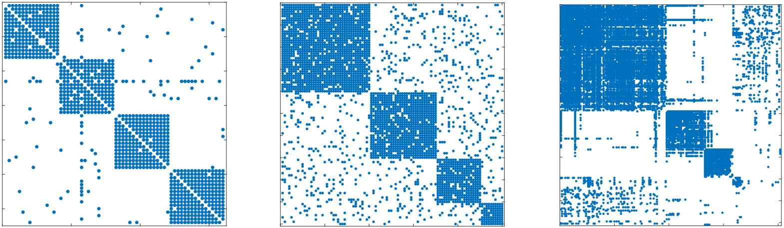
Key idea (Pre-simulation step)

Identification of submatrices.

- Identify relatively dense and relatively sparse submatrices.

Simple test case (left).

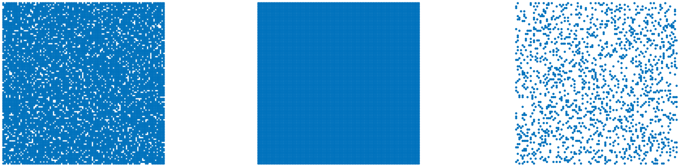
- Four communities of oscillators. Numerous pairwise interactions within each community and few pairwise interactions otherwise.



Key idea (Evaluation step)

Evaluation of defining function.

- For a relatively dense submatrix, the main component corresponds to a classical subsystem, which is resolved in an efficient manner by precomputations (see first part of the talk). The contributions of zero coefficients are compensated.



dense submatrix = full matrix − sparse submatrix

- For a relatively sparse submatrix, the straightforward summation of non-zero coefficients is used.

Numerical illustrations

General setting. Time integration of Kuramoto systems on graphs.

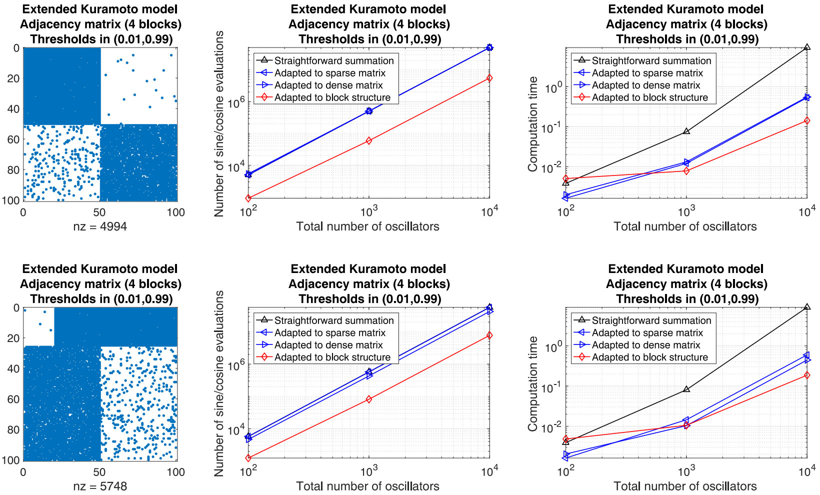
Specific setting. Random generation of adjacency matrices through certain thresholds per block. Evaluation of the defining functions by straightforward summation or approaches adapted to sparse matrices, dense matrices, and block matrices.

- Illustration of the adjacency matrix.
- Comparison of the numbers of sine and cosine evaluations versus the total numbers of oscillators.
- Comparison of the computation times.

Observations. The obtained results confirm that the novel approach is beneficial for a higher number of oscillators, where the evaluation of functions and the computation of sums are expected to be the most time consuming components.

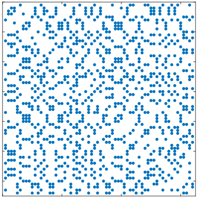
Numerical illustrations

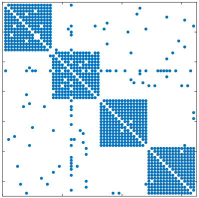
Block matrices involving two dense blocks.

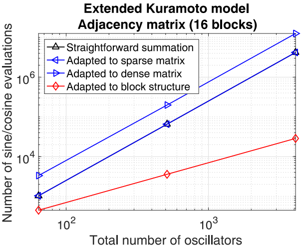


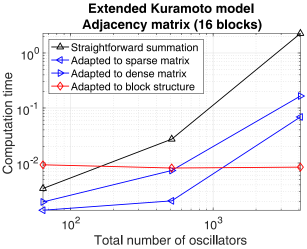
Numerical illustrations

Block matrix involving four dense blocks. A more realistic adjacency matrix describes the interactions of four communities of oscillators.





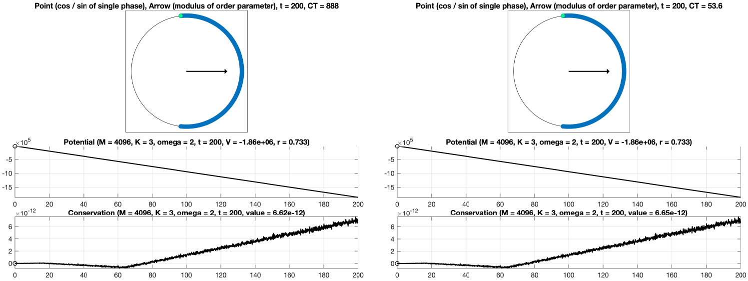




Numerical illustrations

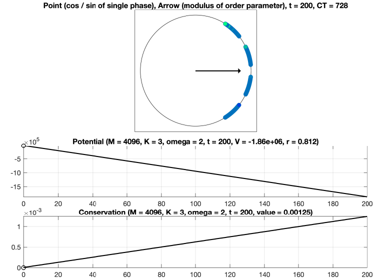
Numerical integration of a Kuramoto model on a graph comprising four communities. Consideration of the common uniform scaling.

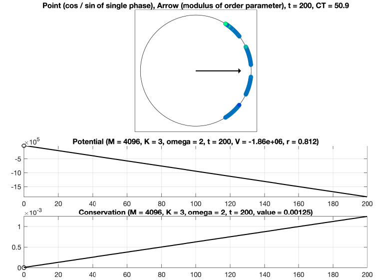
- Evaluation of the right-hand side by straightforward summation.
- Employing the block structure of the associated adjacency matrix and using the precomputation of sums permits a significant reduction of the computation time!



Numerical illustrations

Corresponding results for a non-uniform scaling. Synchronisation within four communities is observed. Due to the lack of symmetry of the system, the conservation property does not hold. Again, the computation time is significantly reduced.





Summary and open questions

Summary.

- A novel approach for the reliable and efficient evaluation of the defining functions permits numerical simulations for large-scale dynamical systems on graphs.

Open questions.

- Suitable approximations of the defining functions to enhance more general applicability.

Thank you!