

# Numerical Linear Algebra for Computational Science and Information Engineering

## Lecture 00 Introduction

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# Outline I

- 1 Numerical linear algebra:  
The "Why?", the "What?" and "What's next?" 1
- 2 Computational mathematics @ TUM 4
- 3 Class overview 7
- 4 Homework assignment 14

# Numerical linear algebra: The "Why?", the "What?" and "What's next?"

# Why do we need numerical linear algebra?

## Prevalence of linear algebra in research and industry:

- Scientific computing (often explicitly related to problems of linear algebra)
- Simulations (e.g., discretized PDEs, ODEs, DAEs, ...)
- Machine learning (e.g., PCA, RKHS, ...)
- Optimization

## Methods taught in linear algebra:

- Solving linear systems: Cramer's rule and Gaussian elimination
- Matrix factorizations: Cholesky, LU and QR
- Eigenvalue problems: Root-finding of characteristic polynomials

## Limitations of methods taught in linear algebra:

- **No general exact method for eigenvalues of matrices** larger than  $4 \times 4$
- **Computational infeasibility** of analytical methods **for large systems**
- **Numerical instability** leading to significant **errors**
- **Inability to handle special structures** (e.g., sparsity, implicitness)

**Need for methods to solve challenging problems  
efficiently**

# What is numerical linear algebra?

## What does numerical linear algebra (NLA) address:

- Efficient algorithms for large-scale problems of linear algebra
- Techniques for maintaining numerical stability and accuracy
- Methods for exploiting matrix structure (e.g., sparsity, symmetry, low-rank)
- Matrix-free formulations for implicit operators
- Error analysis and conditioning

## Scope of NLA:

- Focuses on both theoretical analysis (e.g., convergence, conditioning and stability) and practical implementation.
- Incorporates aspects of performance and computer architecture for method development, e.g.,
  - Repurposing solvers into preconditioners for higher performance.
  - Designing sparse data structures and BLAS kernels to optimize memory usage.

## Key branches of NLA:

- **Direct methods** vs **iterative methods** (stationary vs Krylov)
- **Dense matrices** vs **sparse matrices** and **matrix-free operators**

# What's coming next in numerical linear algebra?

Recent developments in NLA research show promise for significant performance improvements, but face challenges in widespread adoption:

- ▶ **Randomization:** Randomly reduces problem dimensions while preserving inherent structure with high probability. Associated challenges are
  - Ensuring convergence and assessing stability.
  - Defining and implementing reliably amortized sketching procedures.
- ▶ **Communication avoidance:** Redesigns algorithms to minimize data movement between processors or memory hierarchies. Challenges are
  - Maintaining numerical stability with reduced communication.
- ▶ **Mixed precision:** Utilizes different numerical precisions within a single algorithm to optimize performance. Associated challenges are
  - Ensuring overall stability and accuracy with lower precision components.
  - Developing adaptive strategies for precision selection.
- ▶ **Extension of state-of-the art methods to tensor data:** Assessing convergence and stability when using low-rank approximation of tensor data, e.g., Tucker and Tensor-Train formats.

# Computational mathematics @ TUM

# Computational mathematics @ TUM, Campus Heilbronn

- ▶ Chair of COmputational MAtematics (COMA) @ TUM: Prof. **Hartwig Anzt**
  - Professor @ TUM since 01/2024
  - Director of the Innovative Computing Lab @ University of Tennessee (2022-23)
  - Junior Professor @ KIT (2021-22)
- ▶ Recent and ongoing PhD theses directed by Hartwig:
  - Symbolic LU factorizations on GPUs (**Tobias Ribizel**, ongoing)
  - Scalable domain decomposition on GPUs (**Fritz Göbel**, ongoing)
  - Numerical compression in scientific computing (**Thomas Grützmacher**, ongoing)
  - Mixed precision algebraic multigrids on GPUs (**Yu-Hsiang Mike Tsai**, 2024)
  - Asynchronous and batched iterative solvers on GPUs (**Pratik Nayak**, 2023)
- ▶ Ongoing projects in COMA:
  - **Ginkgo**: Portable high-performance numerical linear algebra library
  - **Sparse BLAS**: Basic linear algebra subprograms for sparse matrices
  - **ICON**: Large legacy codebase for climate modeling
  - **OGL/OpenFOAM**: Large legacy codebase for computational fluid dynamics
  - **MicroCARD**: Numerical modeling of cardiac electrophysiology
  - **PDExa**: Optimized software methods and technologies for PDEs
  - **nekRS**: Fast and scalable computational fluid dynamics software package



# Computational mathematics @ TUM, Campus Heilbronn, cont'd<sub>1</sub>

## ► Course Instructor:



**Nicolas Venkovic**, Postdoc. in COMA @ TUM

- Postdoctoral Researcher @ TUM since 07/2024
- PhD in Applied Mathematics & Scientific Computing @ Cerfacs (09/2023)
- MSE in Applied Mathematics & Statistics @ Johns Hopkins University (2018)

► Recent and ongoing research efforts (see [venkovic.github.io/research](https://venkovic.github.io/research)):

- **Fast Convolution Kernels (Fourier, Walsh-Hadamard, ...)**
- **Randomized Short-Recurrence Iterative Methods to Approximate:**
  - Matrix Inverses, Eigenpairs, Low-rank and Non-Negative Factorizations
- **Applications:**
  - Stochastic Preconditioning, Matrix Recovery, Parallelization, ...

# Computational mathematics @ TUM, Campus Heilbronn, cont'd<sub>2</sub>

## ► Teaching Assistant:



### **Amir Bouslama**, Master student @ TUM

- Master student in Information Engineering @ TUM since Winter 2025/26
- BSc in Information Engineering @ TUM (Summer 2025)

## ► Responsibilities:

- **Exercise** (Problem Sets) Sessions + **Practice** (Julia) Sessions  
1 Session per 3 Meetings
- **Grading**

## ► Research interests:

- **Numerical Software and Simulation**

# Class overview

# Objectives

Upon completion of the class, students should:

- ▶ Understand why numerical linear algebra (NLA) is essential in practice, and what it encompasses.
- ▶ Be familiar with the challenges of the main problems and procedures of NLA, such as orthogonalization, least-squares solving, factorization, linear solving, preconditioning, eigenvalue solving, ...
- ▶ Understand the definitions, implementations and main properties of the methods presented in class for solving these problems.
- ▶ Recognize some pathological behaviors of these methods and be able to explain unwanted numerical behaviors.
- ▶ Know the strengths and limits of the presented methods, and know when to use them in practice.
- ▶ Have the foundational background to explore methods for solving NLA problems beyond those covered in class.

# Content

- ▶ We will cover the following core topics:
  - Lecture 01: Essentials of linear algebra
  - Lecture 02: Essentials of the Julia language
  - Lecture 03: Floating-point arithmetic and error analysis
  - Lecture 04: Direct methods for dense linear systems
  - Lecture 05: Sparse data structures and basic linear algebra subprograms
  - Lecture 06: Introduction to direct methods for sparse linear systems
  - Lecture 07: Orthogonalization and least-squares problems
  - Lecture 08: Basic iterative methods for linear systems
  - Lecture 09: Basic iterative methods for eigenvalue problems
  - Lecture 10: Locally optimal block preconditioned conjugate gradient
  - Lecture 11: Arnoldi and Lanczos procedures
  - Lecture 12: Jacobi-Davidson method
  - Lecture 13: Krylov subspace methods for linear systems
  - Lecture 14: Preconditioned iterative methods for linear systems
  - Lecture 15: Restarted Krylov subspace methods
  - Lecture 16: Elements of randomized numerical linear algebra
  - Lecture 17: Introduction to communication-avoiding algorithms
  - Lecture 18: Matrix function evaluation

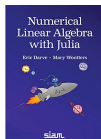
## Content, cont'd

- ▶ If time permits, additional lectures may be picked among the following based on students' interests:
  - Lecture E1: Multigrid methods and domain decomposition
  - Lecture E2: Multilinear algebra and tensor decompositions
  - Lecture E3: Introduction to mixed precision algorithms
- ▶ The duration of a lecture is not tied to a single class period. Some lectures will span less than one class, while others will cover multiple meetings. Several lectures can be covered within one meeting.
- ▶ Most lectures will begin by establishing formal foundations, and some will be followed by practice sessions using **Julia notebooks** and/or **problem sets** to test, visualize, and deepen your understanding of the methods and concepts introduced.

# Reading material

## ► Main references:

- **Lecture slides**, **Julia notebooks** and **problem sets** uploaded gradually on [Moodle](#), throughout the semester.  
Content also uploaded at [venkovic.github.io/NLA-for-CS-and-IE](https://venkovic.github.io/NLA-for-CS-and-IE).



Darve, E., & Wootters, M. (2021). Numerical Linear Algebra with Julia. Society for Industrial and Applied Mathematics (SIAM).<sup>†</sup>

- GitHub repository:  
[https://github.com/EricDarve/numerical\\_linear\\_algebra](https://github.com/EricDarve/numerical_linear_algebra)

## ► Most used supplemental reference #1:

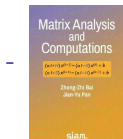


Saad, Y. (2003). Iterative Methods for Sparse Linear Systems. Society for Industrial and Applied Mathematics (SIAM).<sup>†</sup>

<sup>†</sup> SIAM members get 30% off book prices. SIAM membership is free for students.

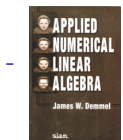
# Reading material, cont'd<sub>1</sub>

## ► Most used supplemental reference #2



Bai, Z. Z., & Pan, J.-Y. (2021). Matrix Analysis and Computations. Society for Industrial and Applied Mathematics (SIAM).<sup>†</sup>

## ► Other useful supplemental references:



Demmel, J. W. (1997). Applied Numerical Linear Algebra. Society for Industrial and Applied Mathematics (SIAM).<sup>†</sup>



Golub, G. H., & Van Loan, C. F. (2013). Matrix Computations. JHU press.

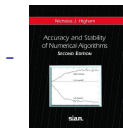
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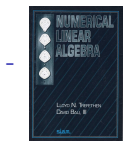
## Reading material, cont'd<sub>2</sub>



- Greenbaum, A. (1997). Iterative Methods for Solving Linear Systems. Society for Industrial and Applied Mathematics (SIAM).<sup>†</sup>



- Higham, N. J. (2002). Accuracy and Stability of Numerical Algorithms. Society for Industrial and Applied Mathematics (SIAM).<sup>†</sup>



- Trefethen, L. N., & Bau, D. (2022). Numerical Linear Algebra. Society for Industrial and Applied Mathematics (SIAM).<sup>†</sup>

<sup>†</sup> SIAM members get 30% off book prices. SIAM membership is free for students.

# Course evaluation

## ► Final exam (determines base grade):

14:00-15:30  
Monday, 16 February 2025  
Campus Heilbronn

- Questions in relation to the homework problems, material presented in class, and practice sessions.

## ► Homework policy:

- Submit your solution to one problem per lecture.
- Deadline: 2 weeks after the end of the lecture.
- Regular submissions upgrade the final grade by one step.
  - Example: 2.0 becomes 1.7.
  - Notes: This upgrade applies to passing grades only.  
1.0 remains the highest possible grade.

# Course evaluation

## ► Retake exam:

14:00-15:30  
Wednesday, 1 April 2025  
Campus Heilbronn

- Questions in relation to the homework problems, material presented in class, and practice sessions.

## ► Homework policy:

- Submit your solution to one problem per lecture.
- Deadline: 2 weeks after the end of the lecture.
- Regular submissions upgrade the final grade by one step.
  - Example: 2.0 becomes 1.7.
  - Notes: This upgrade applies to passing grades only.  
1.0 remains the highest possible grade.

# Homework assignment

# Homework assignment

Send an email to me with the subject line NLA-YourLastName addressing the following points:

- ① Briefly describe your background, if any, in numerical linear algebra, e.g.,
  - Courses taken, practical experience, self-study, ...
- ② Identify a specific area of interest in numerical linear algebra:
  - A problem, method or concept you either work on, want to understand better, or are curious about.
- ③ Regarding the course syllabus:
  - List 2-3 topics you're most excited to learn about.
  - Mention any topics you feel you already have a strong grasp of, or simply would not mind skipping.
- ④ Suggest elective topics, listed in the slides or not, that you'd like to see covered, in case time permits.

**Note:** Your responses could help adapt certain aspects of the course to the class's needs and interests.