



MaRDI – Math, Data, Code

P. Benner, R. Fritze, J. Heiland, C. Himpe, H. Kleikamp, K. Lund,
T. Mitchell, M. Ohlberger, S. Rave, J. Saak, P. Veluvali, et al.

Algorithmic Challenges for Large-Scale Problems

2022–06–14

MaRDI – Mathematical Research Data Initiative

- ▶ **What** is MaRDI?
- ▶ **Why** MaRDI?
- ▶ **How** does MaRDI work?

MaRDI and Me

- ▶ Applied Mathematician
- ▶ Research Topic: Model Reduction
- ▶ Recent Application: Gas Networks
- ▶ Open Science Supporter
- ▶ Pet Peeve: (Un-)Availability
- ▶ MaRDI staff @ WWU Münster



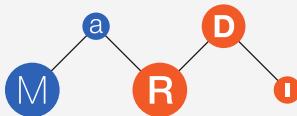
What is MaRDI?

NFDI – Nationale Forschungsdateninfrastruktur

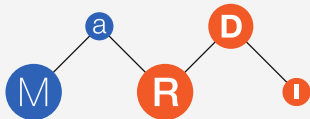
- ▶ Non-profit organisation,
- ▶ for data from science and research,
- ▶ to access, network, and make data usable.
- ▶ Aim: create permanent digital repository.
- ▶ Consists of consortia.



NFDI Consortia



MaRDI Consortium

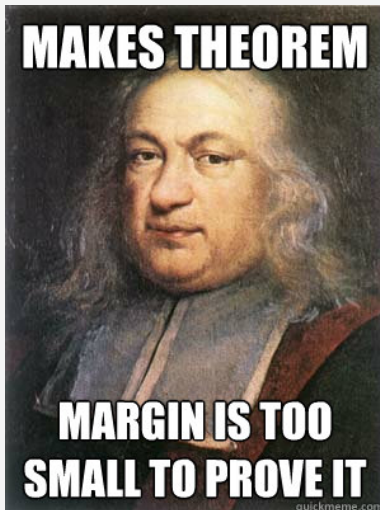


- ▶ Started November 2021
- ▶ 1 of 30 NFDI consortia
- ▶ 15 Institutions plus partners
- ▶ THE math consortium



Why MaRDI?

State of Affairs



Non-Algorithmic Challenges for Large-Scale Problems

- ▶ **Math** Knowledge
- ▶ **CSV Data**
- ▶ **Source Code**

Why should we care (more)?

Math

- ▶ Enter field
- ▶ Efficiently find
- ▶ Keep up-to-date
- ▶ Visibly contribute
- ▶ Handle quantity

$$e^{i\tau} = 1$$

Data

- ▶ Reference results
- ▶ Benchmark data-sets
- ▶ Aggregate data
- ▶ Secondary uses
- ▶ Better visualizations

6, 2, 8, 3, . . .

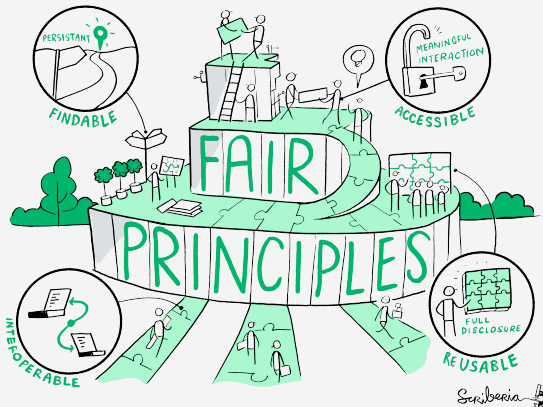
Code

- ▶ Document algorithm
- ▶ Reproduce results
- ▶ Reuse to build upon
- ▶ Reuse to compare against
- ▶ Learn from implementation



FAIR Research Data

- ▶ Findable
- ▶ Accessible
- ▶ Interoperable
- ▶ Reusable



By: Scriberia, CC-BY 4.0, doi:10.5281/zenodo.3332807

(Mathematical) Software

Replicability, Reproducibility, Reusability:

J. Fehr, J. Heiland, C. H., J. Saak:

Best Practices for Replicability, Reproducibility and Reusability of Computer-Based Experiments Exemplified by Model Reduction Software;

AIMS Mathematics 1(3): 261–281, 2016.

doi:10.3934/Math.2016.3.261

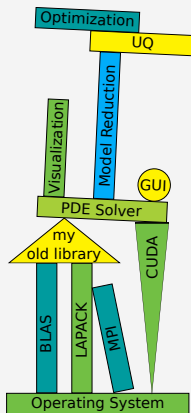
Sustainable Scientific Software:

J. Fehr, C. H., S. Rave, J. Saak:

Sustainable Research Software Hand-Over;

Journal of Open Research Software 9(1): 5, 2021.

doi:10.5334/jors.307



By: S. Rave, CC-BY 4.0,

doi:10.5334/jors.307

How does MaRDI work?

Task Areas

- TA  Task Area 1: **Computer Algebra**
- TA  Task Area 2: **Scientific Computing***
- TA  Task Area 3: **Statistics and Machine Learning**
- TA  Task Area 4: **Interdisciplinary Mathematical Research**
-
- TA  Task Area 5: **The MaRDI Portal**
- TA  Task Area 6: **Data Culture and Community Integration**
- TA  Task Area 7: **Governance and Consortium Management**

TA  **Task Area 2: Scientific Computing**

- ▶ Measure 1: **Algorithm Knowledge Graph**
- ▶ Measure 2: **Open Interfaces**
- ▶ Measure 3: **Benchmark Framework**
- ▶ Measure 4: **CSE Workflows**

Measure 4: CSE Workflows

Goal: Documenting Chained Algorithms

- ▶ Lab notebook for computer experiments
- ▶ Standardized workflow notation
- ▶ Synchronized with engineering sciences
- ▶ Machine readable format
- ▶ Example: *Uncertainty Quantification*

Measure 3: Benchmark Framework

Goal: **Comparing Algorithm Implementations**

- ▶ Fair comparisons and automated testing (specifically for publications)
- ▶ Provide scaffolding (just add algorithms, benchmarks and measures)
- ▶ Local and central service (try at home first, then upload)
- ▶ Assess results (highscores, rankings)
- ▶ For: *Linear Solvers, Matrix Equations, Model Reduction, ...*

Measure 3: Benchmark Framework (cont.)

How does it help fairness and FAIRness?

- ▶ Competitor implementations (**R**)
- ▶ Seamless data handling (**I**)
- ▶ Standard measurements (**A**)
- ▶ Decision aid (**F**)
- ▶ Find the right tool for a job

Measure 2: Open Interfaces

Goal: **Coupling Algorithms Seamlessly**

- ▶ Standard interfaces for numerical libraries
- ▶ Provide interface definitions and wrappers
- ▶ Handle language barriers
- ▶ Coordinate data flow and exchange
- ▶ For: *Linear Solvers, ODE Solvers, PDE Solvers, ...*

Measure 2: Open Interfaces (cont.)

Focus: **Interoperability**

- ▶ Abstraction: problem specific interfaces
- ▶ Intermediate language: C
- ▶ Back-end handles data: via files or memory
- ▶ Long term: language interfaces are generated from specification
- ▶ Example: BLAS / LAPACK → FlexiBLAS

Measure 1: Algorithm Knowledge Graph

Goal: **Contextualize Numerical Algorithms**

- ▶ Easily searchable semantic web of algorithm meta-data
- ▶ Connect algorithms with publications, implementations, problems
- ▶ Build comprehensive and unbiased algorithm meta-data database
- ▶ Community driven expansion and curation
- ▶ For: *Numerical Algorithms*

Measure 1: Algorithm Knowledge Graph (cont.)

- ▶ **What exactly is a knowledge graph?**
→ A list of subject-predicate-object statements.
- ▶ **What are subject, predicate, and object?**
→ All are URIs with meaning, like a URI for “algorithm”.
- ▶ **What makes a knowledge graph powerful?**
→ An enforced ontology.
- ▶ **What is an ontology?**
→ A vocabulary plus a grammar.
- ▶ **Can you give an example statement?**
→ `al:SVD a :algorithm .`

Measure 1: Algorithm Knowledge Graph (cont.)

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 - `https://mardi4nfdi.de/algodata/0.1/algorithm#SVD` a :algorithm .

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Measure 1: Algorithm Knowledge Graph (cont.)

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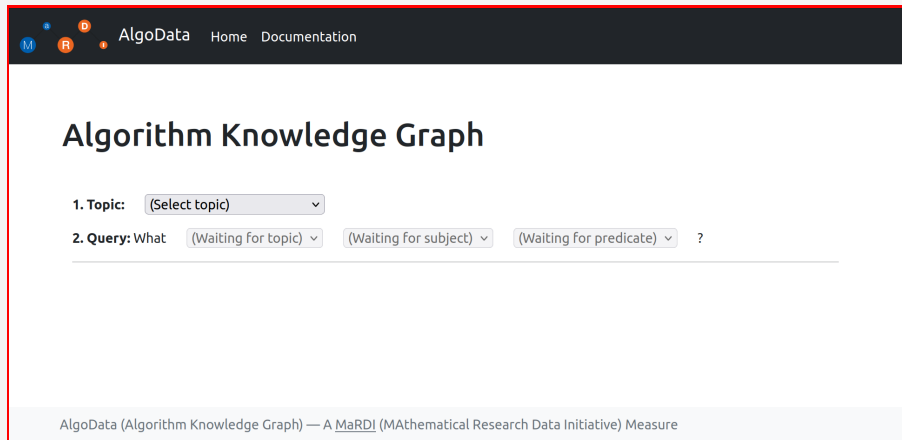
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Measure 1: Algorithm Knowledge Graph (cont.)²

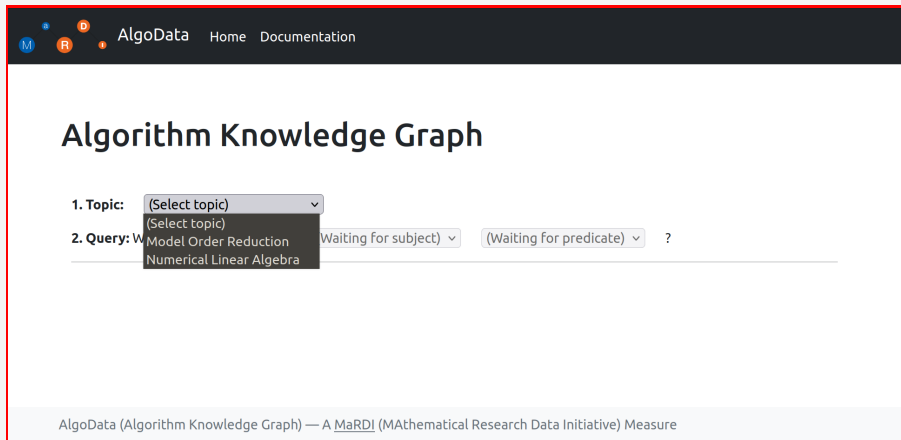
A First Look at the Prototype Front-End

Measure 1: Algorithm Knowledge Graph (cont.)²



The screenshot shows the 'AlgoData' web interface. At the top, there is a navigation bar with the 'AlgoData' logo (a graph with nodes M, R, D) and links for 'Home' and 'Documentation'. The main heading is 'Algorithm Knowledge Graph'. Below this, there are three dropdown menus for search criteria: '1. Topic: (Select topic) v', '2. Query: What (Waiting for topic) v (Waiting for subject) v (Waiting for predicate) v', and a question mark '?' to the right. A horizontal line is positioned below the search criteria. At the bottom of the interface, there is a footer text: 'AlgoData (Algorithm Knowledge Graph) — A MaRDI (MAtheMatical Research Data Initiative) Measure'.

Measure 1: Algorithm Knowledge Graph (cont.)²

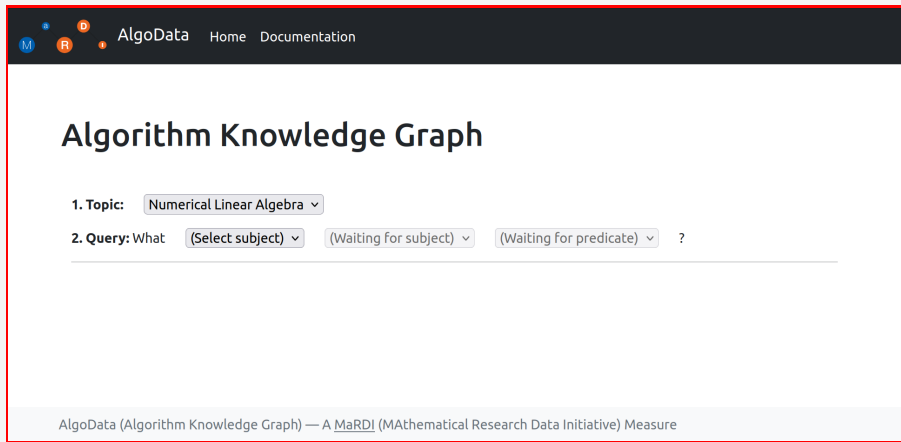


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- 1. Topic:** A dropdown menu with '(Select topic)' selected.
- 2. Query:** A search input field containing 'Waiting for subject'. To its right is another dropdown menu with '(Waiting for predicate)' selected, followed by a question mark '?'.
- Below the search input, a dropdown menu is open, showing two options: 'Model Order Reduction' and 'Numerical Linear Algebra'.

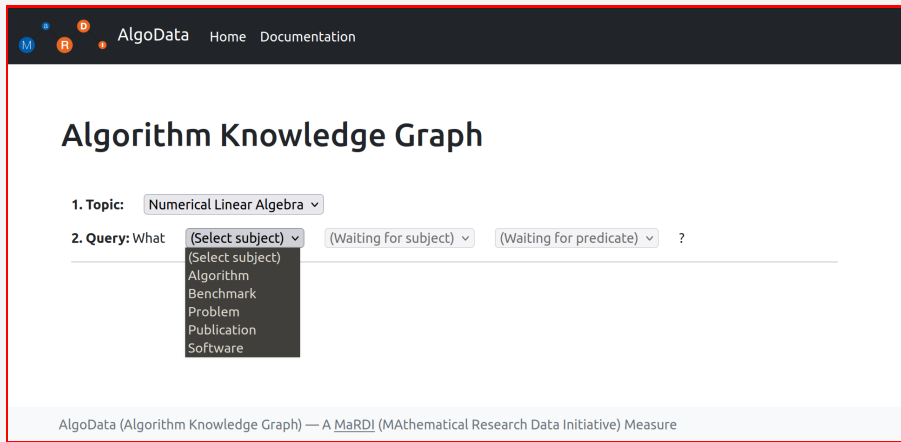
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Measure 1: Algorithm Knowledge Graph (cont.)²



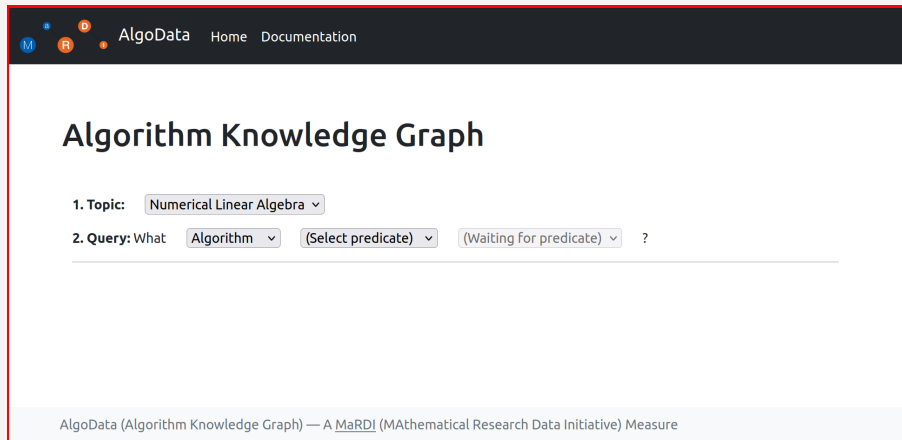
The screenshot shows the 'AlgoData' website interface. The navigation bar includes 'AlgoData', 'Home', and 'Documentation'. The main heading is 'Algorithm Knowledge Graph'. Below this, there are three dropdown menus for filtering: '1. Topic: Numerical Linear Algebra', '2. Query: What (Select subject)', and '(Waiting for subject)'. There is also a '(Waiting for predicate)' dropdown and a question mark. A horizontal line is drawn below the query filters. At the bottom of the page, a footer reads: 'AlgoData (Algorithm Knowledge Graph) — A MaRDI (Mathematical Research Data Initiative) Measure'.

Measure 1: Algorithm Knowledge Graph (cont.)²



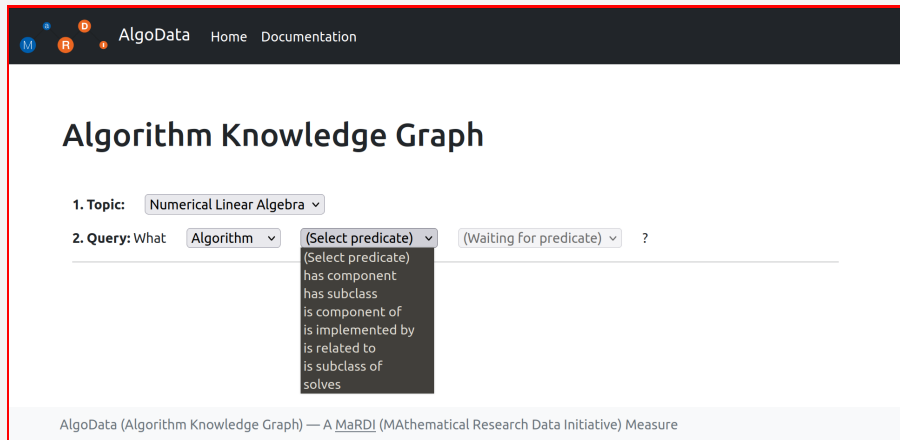
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Measure 1: Algorithm Knowledge Graph (cont.)²



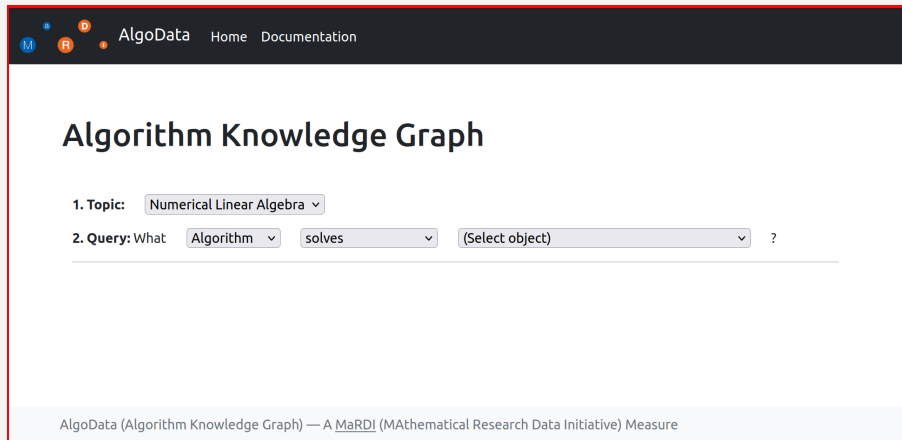
The screenshot shows the 'AlgoData' website interface. At the top, there is a navigation bar with the text 'AlgoData Home Documentation' and a small network diagram on the left. The main content area features a large heading 'Algorithm Knowledge Graph'. Below this, there are two rows of interactive elements. The first row is labeled '1. Topic:' and contains a dropdown menu with 'Numerical Linear Algebra' selected. The second row is labeled '2. Query: What' and contains three dropdown menus: 'Algorithm', '(Select predicate)', and '(Waiting for predicate)', followed by a question mark. A horizontal line is positioned below these dropdowns. At the bottom of the page, there is a footer with the text 'AlgoData (Algorithm Knowledge Graph) — A MaRDI (Mathematical Research Data Initiative) Measure'.

Measure 1: Algorithm Knowledge Graph (cont.)²



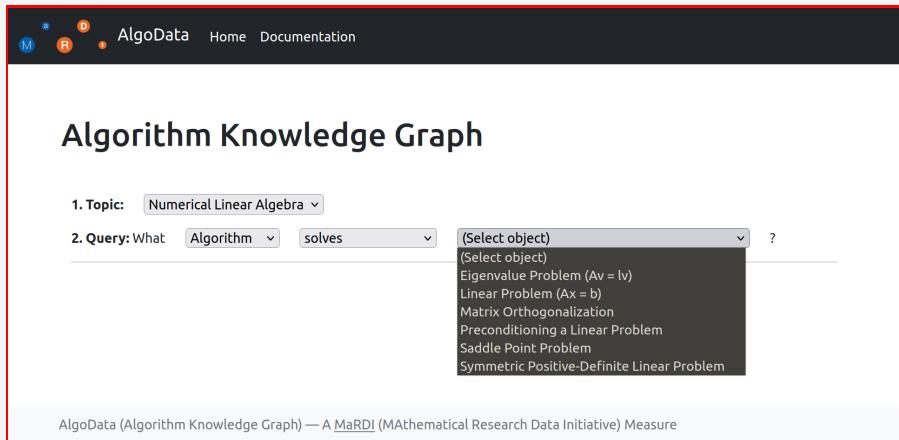
The screenshot shows the 'AlgoData' web interface. At the top, there is a navigation bar with 'AlgoData', 'Home', and 'Documentation' links. Below the navigation bar, the main heading is 'Algorithm Knowledge Graph'. The search form consists of two rows. The first row is labeled '1. Topic:' and has a dropdown menu with 'Numerical Linear Algebra' selected. The second row is labeled '2. Query: What' and has three dropdown menus: 'Algorithm', '(Select predicate)', and '(Waiting for predicate)'. The '(Select predicate)' dropdown is open, showing a list of predicates: '(Select predicate)', 'has component', 'has subclass', 'is component of', 'is implemented by', 'is related to', 'is subclass of', and 'solves'. At the bottom of the interface, there is a footer text: 'AlgoData (Algorithm Knowledge Graph) — A MaRDI (M^Athematical R^Esearch D^Ata I^Nitiative) Measure'.

Measure 1: Algorithm Knowledge Graph (cont.)²



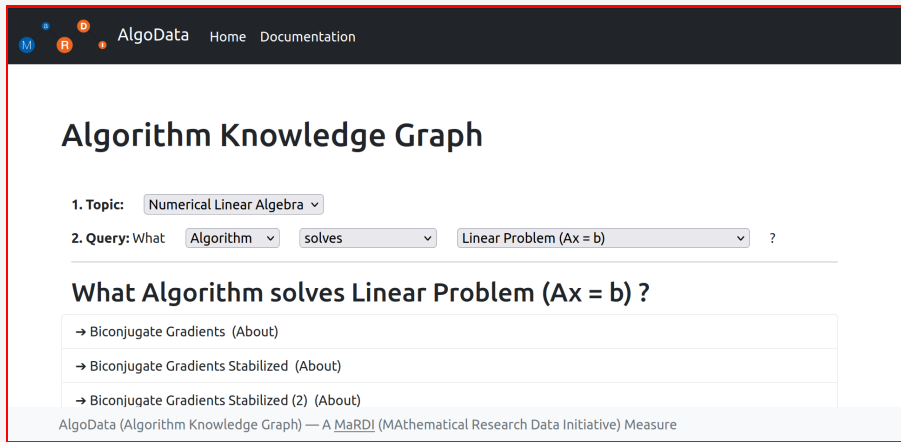
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Measure 1: Algorithm Knowledge Graph (cont.)²



The screenshot shows the AlgoData web interface. At the top, there is a navigation bar with the text "AlgoData Home Documentation" and a small graph icon. The main heading is "Algorithm Knowledge Graph". Below this, there are two search criteria: "1. Topic: Numerical Linear Algebra" and "2. Query: What Algorithm solves". A dropdown menu is open for the "What" field, showing a list of objects: "(Select object)", "Eigenvalue Problem ($Av = lv$)", "Linear Problem ($Ax = b$)", "Matrix Orthogonalization", "Preconditioning a Linear Problem", "Saddle Point Problem", and "Symmetric Positive-Definite Linear Problem". A question mark icon is visible to the right of the dropdown. At the bottom of the interface, there is a footer text: "AlgoData (Algorithm Knowledge Graph) — A MaRDI (M^Athematical R^Esearch D^Ata I^Nitiative) Measure".

Measure 1: Algorithm Knowledge Graph (cont.)²



The screenshot shows the AlgoData website interface. At the top, there is a navigation bar with the logo (M, R, D) and links for Home and Documentation. The main heading is "Algorithm Knowledge Graph". Below this, there is a search form with three dropdown menus: "1. Topic: Numerical Linear Algebra", "2. Query: What Algorithm solves Linear Problem (Ax = b) ?". Below the search form, there is a list of results: "→ Biconjugate Gradients (About)", "→ Biconjugate Gradients Stabilized (About)", and "→ Biconjugate Gradients Stabilized (2) (About)". At the bottom of the screenshot, there is a footer that reads "AlgoData (Algorithm Knowledge Graph) — A MaRDI (MAtheMatical Research Data Initiative) Measure".

Measure 1: Algorithm Knowledge Graph (cont.)²

What Algorithm solves Linear Problem ($Ax = b$) ?

- Biconjugate Gradients (About)
- Biconjugate Gradients Stabilized (About)
- Biconjugate Gradients Stabilized (2) (About)
- Biconjugate Gradients Stabilized (l) (About)
- Cholesky Decomposition (About)
- Gradient Descent (About)
- Generalized Minimal Residual (About)
- Jacobi Method (About)
- LU decomposition (About)
- Crout Inner Product Gaussian Elimination (About)

AlgoData (Algorithm Knowledge Graph) — A MaRD! (M^Athematical R^Esearch D^Ata I^Nitiative) Measure

Measure 1: Algorithm Knowledge Graph (cont.)²

Cholesky Decomposition ↗

... **has subclass:** [gaxpy Cholesky Factorization](#) (About)

... **has subclass:** [Outer Product Cholesky Factorization](#) (About)

... **is analyzed in:** [Higham \(2002\) Accuracy and Stability of Numerical Algorithms](#)

... **is implemented by:** [Armadillo - C++ library for linear algebra & scientific computing](#) (About)

... **is implemented by:** [ARMAS - Another Rewrite of Matrix Algebra Subroutines](#) (About)

... **is implemented by:** [Eigen](#) (About)

... **is implemented by:** [Ginkgo - A high performance numerical linear algebra library](#) (About)

... **is implemented by:** [LAPACK - Linear Algebra PACKage](#) (About)

... **is implemented by:** [MAGMA - Matrix Algebra on GPU and Multicore Architectures](#) (About)

... **is implemented by:** [PLASMA - Parallel Linear Algebra Software for Multicore Architectures](#) (About)

AlgoData (Algorithm Knowledge Graph) — A MaRDI (M^Athematical R^Esearch D^Ata I^Nitiative) Measure

Measure 1: Algorithm Knowledge Graph (cont.)²

... **is invented in:** [Benoit \(1924\) Note Sur Une Méthode de Résolution des équations Normales Provenant de L'Application de la Méthode des Moindres Carrés a un Système D'équations Linéaires en Nombre Inférieur a Celui des Inconnues. — Application de la Méthode a la Résolution D'un Système Défini D'équations Linéaires](#)

... **is reviewed in:** [Atkinson \(1991\) An Introduction to Numerical Analysis](#)

... **is reviewed in:** [Epperson \(2013\) An Introduction to Numerical Methods and Analysis](#)

... **is reviewed in:** [Golub, Van Loan \(2013\) Matrix Computations](#)

... **is reviewed in:** [Greenbaum \(1997\) Iterative Methods for Solving Linear Systems](#)

... **is reviewed in:** [Quarteroni, Sacco, Saleri \(2007\) Numerical Mathematics](#)

... **is reviewed in:** Trefethen, Bau (1997) Numerical Linear Algebra

... **is studied in:** [Volkov, Demmel \(2008\) Benchmarking GPUs to tune dense linear algebra](#)

... **solves:** Linear Problem ($Ax = b$) (About)

... **uses:** Minimum Degree Algorithm (About)

AlgoData (Algorithm Knowledge Graph) — A [MaRDI](#) (M^Athematical R^Esearch D^Ata I^Nitiative) Measure

MaRDI and You

▶ **Portal:** portal.mardi4nfdi.de

▶ **Twitter:** @mardi4nfdi

▶ **Newsletter:** Coming Soon

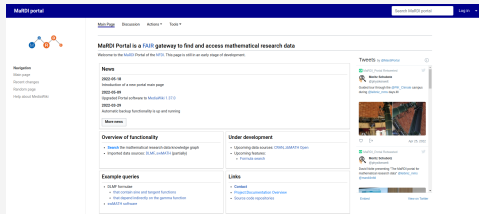
▶ **Reading:**

- ▶ C. Görgen, R. Sinn:

Mathematik in der Nationalen Forschungsdateninfrastruktur;
DMV Mitteilungen 29(3): 122-123, 2021. doi:10.1515/dmvm-2021-0049

- ▶ P. Benner, M. Burger, D. Göddeke, C. Görgen, C. H., M. Hintermüller, J. Heiland, T. Koprucki, M. Ohlberger, S. Rave, M. Reidelbach, J. Saak, A. Schöbel, K. Tabelow, M. Weber:

Die Mathematische Forschungsdateninitiative in der NFDI: MaRDI;
GAMM-Rundbrief 2022(1): 40-43, 2022.
gamm-ev.de/publikationen/gamm-rundbriefe



The screenshot shows the MaRDI Portal homepage. The header includes navigation tabs for Home, Discussion, Actions, and Tools. The main content area is titled 'MaRDI Portal is a **FAIR** gateway to find and access mathematical research data'. Below this, there are sections for 'News' (with dates from 2022-05-18 to 2022-05-25), 'Overview of functionality' (listing search, data source, and software), 'Under development' (listing updates, updates, and software), 'Example queries' (listing CLM, model, and software), and 'Links' (listing Contact, Project, and Source code repositories). A sidebar on the right shows a Twitter feed.

1st MaRDI Workshop on Scientific Computing

2022-10-26 – 2022-10-28

Münster

<https://workshop.mardi.ovh>

Summary

- ▶ MaRDI: Make math FAIR
- ▶ Knowledge Graph (TA2-M1)
- ▶ Open Interfaces (TA2-M2)
- ▶ Benchmark Framework (TA2-M3)
- ▶ CSE Workflows (TA2-M4)
- ▶ Slides at: <https://himpe.science>

<https://mardi4nfdi.de>

Supported by the German Research Foundation (Deutsche Forschungsgemeinschaft), No.: 460135501.
NFDI 29/1 “MaRDI – Mathematische Forschungsdateninitiative”.

My Questions:

- ▶ Do you have a mathematical research data story?
- ▶ Do you have an issue MaRDI could improve?
- ▶ How can CRC1456 and MaRDI cooperate?