

NONLINEARSOLVE.jl: HIGH-PERFORMANCE AND ROBUST SOLVERS FOR SYSTEMS OF NONLINEAR EQUATIONS IN JULIA*

AVIK PAL[†], FLEMMING HOLTORF , AXEL LARSSON , TORHEL LOMAN , UTKARSH , FRANK SCHÄFER , QINGYU QU , ALAN EDELMAN , AND CHRIS RACKAUCKAS[‡]

Abstract. Efficiently solving nonlinear equations underpins numerous scientific and engineering disciplines, yet scaling these solutions for complex system models remains a challenge. This paper presents `NonlinearSolve.jl` – a suite of high-performance open-source nonlinear equation solvers implemented natively in the Julia programming language. `NonlinearSolve.jl` distinguishes itself by offering a unified API that accommodates a diverse range of solver specifications alongside features such as automatic algorithm selection based on runtime analysis, support for GPU-accelerated computation through static array kernels, and the utilization of sparse automatic differentiation and Jacobian-free Krylov methods for large-scale problem-solving. Through rigorous comparison with established tools such as `Sundials` and `MINPACK`, `NonlinearSolve.jl` demonstrates unparalleled robustness and efficiency, achieving significant advancements in solving benchmark problems and challenging real-world applications. The capabilities of `NonlinearSolve.jl` unlock new potentials in modeling and simulation across various domains, making it a valuable addition to the computational toolkit of researchers and practitioners alike.

Key words. Nonlinear Systems, Root Finding, Sparsity Detection, Automatic Differentiation, JuliaLang

1. Introduction. Nonlinear equations are ubiquitous across the sciences, governing the behavior of complex systems in domains ranging from physics to biology to machine learning. Solving steady state (or fixed-point) equations, implicit Ordinary Differential Equation (ODE) [1], semi-explicit Differential Algebraic Equations (DAEs), boundary value differential equations [2, 3, 4, 5], and memory-efficient deep learning [6, 7, 8, 9] all boil down to solving nonlinear equations. Despite their prevalence in real-world problems, finding solutions to nonlinear equations at scale remains a major challenge.

This paper presents `NonlinearSolve.jl` - an open-source, high-performance nonlinear equation-solving framework implemented in the Julia Programming Language [10]. `NonlinearSolve.jl` provides a flexible, easy-to-use interface for specifying and solving general nonlinear equations. Under the hood, it employs various state-of-the-art techniques such as automatic sparsity exploitation, fast automatic differentiation, and jacobian-free methods to solve systems at scale reliably. `NonlinearSolve.jl` is part of the **Scientific Machine Learning (SciML) package ecosystem of Julia**¹ and is, in turn, extended by various packages to solve domain-specific problems. The key capabilities and contributions of `NonlinearSolve.jl` include:

- Unified API for Rapid Experimentation with Nonlinear Solver Options: Users can seamlessly switch between solver algorithms (including the same algorithm from different software packages), line search methods, trust region schemes, automatic-differentiation backends, linear solvers (including Krylov methods), and sparsity detection algorithms.

*Submitted to the editors.

Funding: The authors would like to thank DARPA for funding this work through the Automating Scientific Knowledge Ex-traction and Modeling (ASKEM) program, Agreement No. HR0011262087. The views, opinions and/or findings expressed are those of the authors and should not be interpreted as representing the official views or policies of the Department of Defense or the U.S. Government.

[†]CSAIL MIT, Cambridge, MA (avikpal@mit.edu, <https://avik-pal.github.io>).

[‡]CSAIL MIT, Cambridge, MA (crackauc@mit.edu, <https://www.chrisrackauckas.com/>).

¹<https://sciml.ai/>

- Smart Polyalgorithmic Solver Selection for Robustness: Automated runtime checks select appropriate internal solver methods and parameters, balancing speed and reliability.
- High-performance Algorithms for Small Problems: Specialized non-allocating kernels solve small systems extremely efficiently – outperforming existing software.
- Automatic Sparsity Exploitation for Large Systems: Approximation techniques automatically detect sparsity patterns in system Jacobians. Colored sparse matrix computations coupled with sparse linear solvers accelerate both derivative calculations and overall solve times.
- Jacobian-Free Krylov Methods: Matrix-free linear solvers avoid explicit Jacobian materialization, reducing memory overhead and enabling the solution of otherwise computationally infeasible systems.
- Composable Blocks for Building Solvers: All solvers in `NonlinearSolve.jl` are built using a composition of fundamental building blocks – Descent Algorithm, Linear Solver, Jacobian Computation Algorithm, and Globalization Strategy.
- Symbolic Tearing of Nonlinear Systems: `ModelingToolkit.jl` [11] automatically performs tearing of nonlinear systems for `NonlinearSolve.jl` and reduces the computational complexity of solving those systems.

We demonstrate the capabilities of `NonlinearSolve.jl` with several numerical experiments. The software reliably solves 23 nonlinear test problems [Subsection 4.1], outperforming the open-source `Sundials` toolkit and reference MINPACK implementation. Furthermore, we show `NonlinearSolve.jl`'s applicability to large real-world problems by benchmarking it on applications like initializing a DAE battery model [Subsection 4.2] and steady-state Partial Differential Equation (PDE) solving [Subsection 4.3]. `NonlinearSolve.jl` enables fast yet robust nonlinear equation solving on problems where existing tools break down. Its efficiency, flexibility, and seamless GPU support unlock new modeling and simulation capabilities across application domains.

1.1. Comparison to Existing Software. Most existing nonlinear solvers exhibit flexibility, performance, and scalability limitations when applied to real-world nonlinear problems. For example, `Sundials` KINSOL [12, 13] is specialized for implicit ODE solvers, and tricks like Jacobian reuse often fail for simple test problems [Subsection 4.1]. MINPACK [14, 15] forms the base for popular packages like `SciPy` [16] and `MATLAB fsolve` [17]; however, this lacks the support of tools like Automatic Differentiation (AD), sparsity detection, and Krylov methods, is often more than 100 times slower than our solvers [Figure 10] and fails for numerically challenging problems [Subsection 4.2]. PETSc SNES [18] is a specialized set of solvers for large systems in a distributed setup; however, they lack the support for sparse AD and instead can compute sparse Jacobians exclusively via colored finite differencing. `Optimistix` [19] solves systems of nonlinear equations for machine learning-focused applications and, as such, lacks support for any form of sparsity handling that is uncommon in their target domain. We draw much inspiration from pre-existing Julia Packages like `NLsolve.jl` and `NLSolvers.jl` [20]; however, they had similar problems of scalability and lacked specialized linear solvers as evident from their slower relative performance [Section 4]. In contrast to existing software, `NonlinearSolve.jl` is designed to be robust, performant, and scalable in general while having controls to be customized to specific applications

1.2. Domain Specific Extensions of `NonlinearSolve.jl`. In addition to the core framework for solving nonlinear systems, `NonlinearSolve.jl` is extended by

several packages to solve domain-specific problems. These extensions include:

1. `SteadyStateDiffEq.jl`: Enables computing the steady state of dynamical systems. `Catalyst.jl`'s² `tutorials`³ demonstrate how this is used to determine the steady states of a dimerization reaction network.
2. `DeepEquilibriumNetworks.jl`: Utilizes the sensitivity analysis capabilities of `NonlinearSolve.jl` to train deep equilibrium networks [Subsection 2.3].
3. `DiffEqCallbacks.jl`: Provides `ManifoldCallback` for solving semi-explicit ODEs on arbitrary manifolds. `Our tutorials`⁴ demonstrate how `NonlinearSolve.jl` can be used to conserve energy and angular momentum in the Kepler Problem [22].
4. `OrdinaryDiffEq.jl`: Uses `NonlinearSolve.jl` to initialize DAE solves. In Subsection 4.2, we solve the DAE initialization problem for a battery model using `NonlinearSolve.jl`.

2. Mathematical Description. This section introduces the mathematical framework for numerically solving nonlinear problems and demonstrates the built-in support for such problems in `NonlinearSolve.jl`. A nonlinear problem is defined as:

$$(2.1) \quad \text{Find } u^* \text{ s.t. } f(u^*, \theta) = 0$$

where $f : \mathbb{R}^n \times \mathbb{P} \rightarrow \mathbb{R}^n$ and $\theta \in \mathbb{P}$ is a set of fixed parameters. In this paper, we will assume that f is continuous and differentiable⁵. For a more rigorous and detailed discussion on numerical solvers for nonlinear systems, we refer the readers to [23, Chapter 11].

2.1. Numerical Algorithms for Nonlinear Equations. Numerical nonlinear solvers start with an initial guess u_0 and iteratively refine it until a convergence criterion is satisfied, typically, $\|f(u_k, \theta)\|_\infty \leq \text{abstol}$. (where $\|\cdot\|_\infty$ denotes the max-norm). Newton-Raphson is a powerful iterative technique for finding the roots of a continuously differentiable function $f(u, p)$. It iteratively refines an initial guess u_0 using the formula:

$$(2.2) \quad \mathcal{J}_k \delta u_{\text{newton}} = -f(u_k, \theta)$$

$$(2.3) \quad u_{k+1} = u_k + \delta u_{\text{newton}},$$

where \mathcal{J}_k is the Jacobian of $f(u, \theta)$ with respect to u , evaluated at u_k . This method exhibits rapid convergence [23, Theorem 11.2] when the initial guess is sufficiently close to a root. Furthermore, it requires only the function and its Jacobian, making it computationally efficient for many practical applications. Halley's method enhances the Newton-Raphson method, leveraging information from the second total derivative of the function to achieve cubic convergence. It refines the initial guess u_0 using:

$$(2.4) \quad a_k^\gamma = \delta u_{\text{newton}}$$

$$(2.5) \quad \mathcal{J}_k b_k^\gamma = \mathcal{H}_k a_k^\gamma a_k^\gamma$$

$$(2.6) \quad \delta u_{\text{halley}} = (a_k^\gamma \circ a_k^\gamma) \oslash \left(a_k^\gamma + \frac{1}{2} b_k^\gamma \right)$$

$$(2.7) \quad u_{k+1} = u_k + \delta u_{\text{halley}}$$

²`Catalyst.jl` [21] is a package for modeling chemical reaction networks.

³https://docs.sciml.ai/Catalyst/dev/catalyst_applications/nonlinear_solve/#nonlinear_solve

⁴https://docs.sciml.ai/DiffEqDocs/stable/examples/kepler_problem/#The-Kepler-Problem

⁵For Halley's method, we additionally assume twice-differentiability.

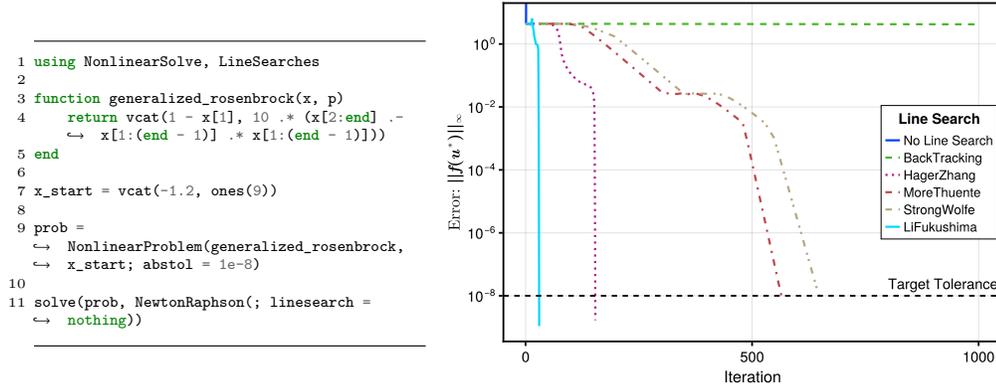


Fig. 1: `NonlinearSolve.jl` allows seamless switching between different line search routines. Instead of `nothing`, we can specify `HagerZhang()`, `BackTracking()`, `MoreThuente()`, `StrongWolfe()`, or `LiFukushimaLineSearch()` to opt-in to using line search. Line search enables `NewtonRaphson` to converge faster on the Generalized Rosenbrock Problem [Equation (2.12)], while it fails to converge without a line search.

where $\mathcal{H}_k = \frac{\partial}{\partial u} \left(\frac{\partial f(u, \theta)}{\partial u} \right)$ is the second total derivative of $f(u, \theta)$ w.r.t. u , evaluated at u_k , and \circ and \oslash denote elementwise multiplication and division respectively. Despite the cubic convergence, the additional cost of computing \mathcal{H}_k often makes Halley’s method practically infeasible.

Multistep Methods are a special class of nonlinear solvers that take multiple intermediate steps between u_k and u_{k+1} to obtain a higher order of convergence. For example, Potra & Pták [24] uses the same Jacobian twice to compute the final descent direction.

$$(2.8) \quad \mathcal{J}_k \delta u_1 = -f(u_k, p)$$

$$(2.9) \quad y_k = u_k + \delta u_1$$

$$(2.10) \quad \mathcal{J}_k \delta u_2 = -f(y_k, p)$$

$$(2.11) \quad u_{k+1} = y_k + \delta u_2.$$

This method provides higher convergence orders without reliance on higher-order derivatives. [25] summarizes other multi-step schemes that provide higher-order convergence using only first-order derivatives. These methods are local algorithms, and their convergence relies on having a good initial guess. We will discuss some techniques to facilitate the global convergence of these methods in the following section.

2.2. Globalization Strategies. Globalization Strategies allow us to enhance the local algorithms described in Subsection 2.1 and ensure global convergence under suitable assumptions [23, Theorem 3.2, 4.5, 4.6].

2.2.1. Line Search. Consider the N -Dimensional Generalized Rosenbrock Function, which is defined as:

$$(2.12) \quad f_i(x, \theta) = \begin{cases} 1 - x_1 & \text{if } i = 1 \\ 10(x_i - x_{i-1}^2) & \text{if } i \in \{2, \dots, N\} \end{cases}$$

If we initialize the problem with $(u_0)_1 = -1.2$, Newton-Raphson fails to converge to the solution [Figure 1]. Line search methods are globalization strategies that avoid

such failures by determining a positive step length α_k given the current iterate u_k and the search direction δu_k

$$(2.13) \quad u_{k+1} = u_k + \alpha_k \delta u_k.$$

The direction is often given by the Newton Descent Direction, Steepest Descent, or one of the Multi-Step Schemes described in [Subsection 2.1](#). The optimal choice for the step length is given by:

$$(2.14) \quad \alpha^* \in \arg \min_{\alpha > 0} \phi(u_k, \alpha) \quad \text{where} \quad \phi(u_k, \alpha) = \frac{1}{2} \|f(u_k + \alpha_k \delta u_k, p)\|^2$$

However, solving a global optimization problem on each step of the iterative nonlinear solver is prohibitively expensive. Instead, practical line search methods rely on selecting a set of candidate step sizes and terminating the search based on certain conditions:

Armijo Rule and Curvature Criteria: The Armijo Rule or Sufficient Decrease criteria states that α_k is acceptable only if there is a sufficient decrease in the objective function:

$$(2.15) \quad \phi(u_k, \alpha) \leq \phi(u_k, 0) + c_1 \alpha \nabla_{u_k} \phi(u_k, 0)^T \delta u_k$$

$$(2.16) \quad = \phi(u_k, 0) + c_1 \alpha \underbrace{f(u_k, \theta)^T \mathcal{J}_k \delta u_k}_{\substack{\text{directional derivative} \\ \text{of } \frac{1}{2}(f)^2 \text{ at } u_k \text{ along } \delta u_k}}$$

Additionally, we use the curvature condition to filter out values for α_k that satisfy sufficient decrease but are very close to the current iterate. This ensures that the algorithm makes reasonable progress at every step.

$$(2.17) \quad \nabla_{u_k} \phi(u_k, \alpha_k)^T \delta u_k \geq c_2 \nabla_{u_k} \phi(u_k, 0)^T \delta u_k$$

where $c_2 \in (c_1, 1)$ and $c_1 \in (0, 1)$. These two conditions are collectively known as the Wolfe Conditions [\[26, 27\]](#).

Strong Wolfe Condition: Strong Wolfe conditions additionally restrict the curvature criteria to restrict the derivative from being too positive:

$$(2.18) \quad \phi(u_k, \alpha) \leq \phi(u_k, 0) + c_1 \alpha \nabla_{u_k} \phi(u_k, 0)^T \delta u_k$$

$$(2.19) \quad |\nabla_{u_k} \phi(u_k, \alpha_k)^T \delta u_k| \geq c_2 |\nabla_{u_k} \phi(u_k, 0)^T \delta u_k|$$

Backtracking Line Search: In this method, we start with an initial step length (typically 1 for most root finding algorithms) and shrink the step length by a (adaptive) factor $\rho \in (0, 1)$. In this case, we automatically ensure that the algorithm is making reasonable progress; hence, we only need to check for the sufficient decrease criteria [\[Equation \(2.16\)\]](#) [\[23, Section 3.1, Sufficient Decrease and Backtracking\]](#).

`NonlinearSolve.jl` supports line search routines for its solvers using the `LineSearches.jl` package [\[20\]](#). In [Figure 1](#), we demonstrate how `NonlinearSolve.jl` provides a uniform API to switch between different line search routines like `BackTracking` [\[23\]](#), `HagerZhang` [\[28\]](#), `MoreThuente` [\[29\]](#), etc. Using line search methods, we successfully solve the generalized Rosenbrock function [\[Equation \(2.12\)\]](#).

2.2.2. Trust Region Methods. As an alternative to using line search as a globalization strategy, trust-region methods restrict the next iterate to lie in a local

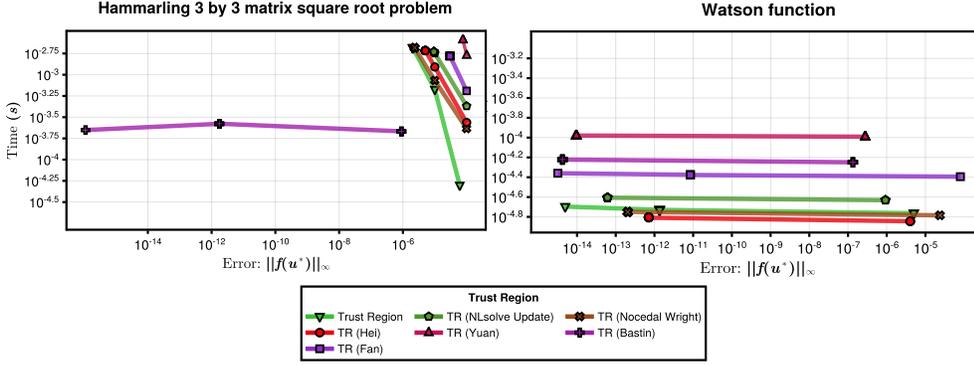


Fig. 2: **Work-Precision Diagrams for Two Instances of the 23 Test Problems:** Trust Region Radius Update Schemes directly affect the convergence of the algorithm, `NonlinearSolve.jl` implements various update schemes and allows switching them with a unified API.

region around the current iterate. These methods estimate a quadratic model for the objective function:

$$(2.20) \quad m_k(\delta u_k) = \frac{1}{2} \|f(x, p)\|^2 + \delta u_k^T \mathcal{J}_k^T f(x, p) + \frac{1}{2} \delta u_k^T \mathcal{J}_k^T \mathcal{J}_k \delta u_k$$

and attempt to solve the following sub-problem:

$$(2.21) \quad \delta u_k^* \in \arg \min_{\delta u_k} m_k(\delta u_k) \quad \text{s.t.} \quad \|\delta u_k\| \leq \Delta_k$$

where Δ_k is the trust region radius at the current iterate k . To perform an update to the current iterate and the trust region radius, we compute the ratio of the actual reduction to the predicted reduction (ρ_k):

$$(2.22) \quad \rho_k = \frac{\|f(x, p)\|^2 - \|f(x + \delta u_k, p)\|^2}{\|f(x, p)\|^2 - \|f(x, p) + \mathcal{J}_k \delta u_k\|^2}$$

If ρ_k is greater than a threshold, i.e., there is a strong agreement between the predicted model and true system, we accept the step and increase the trust-region radius Δ_k . If $0 < \rho_k \ll 1$, we accept the step but keep the trust-region radius unaffected. Otherwise, the trust region is shrunk, and the step is rejected. The exact specification for thresholds for these choices depends on the underlying algorithms being used. `NonlinearSolve.jl` implements additional sophisticated algorithms to update the trust region – Hei [30], Yuan [31], Fan [32], and Bastin [33]. In Figure 2 and Section 4, we demonstrate how different radius update schemes achieve a compromise between the computational cost and solution accuracy.

The trust region subproblem [Equation (2.21)] can be solved approximately using Powell’s Dogleg Method [34], which combines the descent directions from Newton’s Descent ($\delta u_{\text{newton}} = -\mathcal{J}^{-1} f(u, p)$) and the Steepest Descent ($\delta u_{\text{sd}} = -\mathcal{J}^T f(u, p)$). The algorithm proceeds by computing δu_{newton} , and takes the full step if $\|\delta u_{\text{newton}}\| \leq \Delta$. Otherwise, it computes the unconstrained minimizer of the model along the steepest descent direction. If the minimizer is outside the trust region, it accepts the descent vector’s intersection with the hypersphere of radius Δ if $\|\delta u_{\text{sd}}\| \geq \Delta$. Finally, if none of these conditions hold, we compute the interpolated vector $\delta u = (1 - \tau)\delta u_{\text{sd}} + \tau\delta u_{\text{newton}}$, where τ is the largest value $\in (0, 1)$ s.t. $\|\delta u\| \leq \Delta$.

2.3. Sensitivity Analysis. Sensitivity Analysis for nonlinear systems is an integral part of several applications like differentiable physics simulators, deep equilibrium models [6, 8, 9, 35], and optimizing design parameters [36]. Computing gradients for these systems using naive automatic differentiation requires differentiating the nonlinear solve process, which is computationally expensive since it increases the order of differentiation for the solver. Instead, we implement a black-box adjoint method using the implicit function theorem that differentiates the solution directly, independent of the exact solver being used. For a continuous differentiable function $f : \mathbb{R}^n \times \mathbb{P} \rightarrow \mathbb{R}^n$ and $u^* \in \mathbb{R}^n$ and $\theta \in \mathbb{P}$ s.t.:

$$(2.23) \quad f(u^*, \theta) = 0$$

and the Jacobian w.r.t u^* being non-singular, Implicit Function Theorem (IFT) provides an efficient way to compute the Jacobian [37, 38]:

$$(2.24) \quad \frac{du^*}{d\theta} = \left(\frac{\partial f(u^*, \theta)}{\partial u} \right)^{-1} \frac{\partial f(u^*, \theta)}{\partial \theta}$$

`NonlinearSolve.jl` has specialized Krylov Methods to compute the sensitivity efficiently without constructing these Jacobians explicitly using Vector-Jacobian Products (VJP)⁶. Consider the following example, where we use the Forward Mode AD Framework `ForwardDiff.jl` [39] and Reverse Mode AD Framework `Zygote.jl` [40, 41] to differentiate through the solution of $f(u, \theta) = u^2 - p = 0$ with $g(u^*, p) = \sum_i (u_i^*)^2$:

```

1 using NonlinearSolve, SciMLSensitivity, ForwardDiff, Zygote
2
3 # Apply all the operators elementwise using @.
4 f(x, p) = @. x^2 - p
5
6 function solve_nprob(p)
7     prob = NonlinearProblem(f, [1.0, 2.0], p)
8     sol = solve(prob)
9     return sum(abs2, sol.u)
10 end
11
12 p = [2.0, 5.0]
13
14 ForwardDiff.gradient(solve_nprob, p) # Forward Mode
15
16 Zygote.gradient(solve_nprob, p)     # Reverse Mode

```

2.4. Matrix Coloring & Sparse Automatic Differentiation. The Jacobian computation and linear solver are typical bottlenecks for numerical nonlinear equation solvers. If the sparsity pattern of a Jacobian is known, then computing the Jacobian can be done with much higher efficiency [42]. Sparsity patterns for arbitrary programs can be automatically generated using numerical techniques [43, 44] or symbolic methods [45]. Given the sparsity pattern, we can use graph coloring algorithms [46, 47] to compute the matrix colors for the given sparse matrix.

In `NonlinearSolve.jl`, we can compute the sparse Jacobian using both Forward and Reverse Mode AD⁷. AD tools compute the directional derivative using Jacobian-Vector Products (JVPs) $\mathcal{J}u$ for Forward Mode AD and VJPs $\mathcal{J}^T v$ for Reverse Mode AD. To compute a dense $m \times n$ Jacobian, Forward Mode AD (and Finite Differencing) computes n JVPs, and Reverse Mode AD computes m VJPs using the standard basis

⁶We defer the discussion on how to efficiently compute nonlinear solve adjoints for large systems to [9]

⁷Sparse symbolic AD is the most optimal way to compute sparse Jacobians in certain situations. We currently lack the capability for built-in symbolic sparse Jacobians.

vectors. Forward Mode AD fills in the Jacobian one column at a time, and Reverse Mode AD fills in the Jacobian one row at a time. We can chunk multiple JVPs or VJPs together for Jacobians with known sparsity patterns to reduce the overall computation cost. Consider the following sparsity pattern for a Jacobian $\mathcal{J}_{\text{sparse}}$,

$$(2.25) \quad \mathcal{J}_{\text{sparse}} = \begin{bmatrix} \bullet & & & & \\ & \bullet & \bullet & & \\ \bullet & \bullet & & \bullet & \\ & & & & \bullet \\ & & & & \bullet \end{bmatrix}$$

where \bullet denotes the non-zero elements of the Jacobian. To use forward mode AD, we need to compute the column coloring, and for reverse mode⁸ we need the row coloring (which can be obtained by coloring the transposed Jacobian).

$$(2.26) \quad \mathcal{J}_{\text{sparse}}^{(\text{col})} = \begin{bmatrix} \blacktriangleright & & & & \\ & \blacksquare & \blacktriangleright & & \\ \blacktriangleright & \blacksquare & & \blacktriangleright & \\ & & & & \blacklozenge \\ & & & & \blacklozenge \end{bmatrix} \quad \mathcal{J}_{\text{sparse}}^{(\text{row})} = \begin{bmatrix} \blacksquare & & & & \\ & \blacksquare & \blacksquare & & \\ \blacklozenge & \blacklozenge & & & \\ & & & \blacksquare & \\ & & & & \blacksquare \end{bmatrix}$$

Matrix Coloring⁹ allows us to avoid perturbation confusion when we perturb multiple rows/columns of the same color together. For example, in Forward Mode AD perturbing the columns with color \blacktriangleright , we get $[u_1 + \varepsilon, u_2, u_3 + \varepsilon, u_4 + \varepsilon, u_5]$ ($a + \varepsilon$ denotes a Dual number). Propagating this vector, we obtain the result $[v_1 + \delta_1\varepsilon, \dots, v_5 + \delta_5\varepsilon]$. Since all the columns of the Jacobian with the same color are non-overlapping, we can uniquely map the partials to the Jacobian entries: $(\mathcal{J}_{\text{sparse}})_{11} = \delta_1$, $(\mathcal{J}_{\text{sparse}})_{23} = \delta_2$, $(\mathcal{J}_{\text{sparse}})_{34} = \delta_3$, $(\mathcal{J}_{\text{sparse}})_{41} = \delta_4$, and trivially from the sparsity pattern $\delta_5 = 0$. For reverse mode, we proceed similarly, except the perturbation is now on the output. Hence, to compute $\mathcal{J}_{\text{sparse}}^{(\text{col})}$, we need to perform 3 JVPs (once each for \blacktriangleright , \blacksquare , and \blacklozenge) compared to 5 JVPs for a 5×5 dense Jacobian. Similarly, since reverse mode materializes the Jacobian one row at a time, we need 2 VJPs (once each for \blacksquare , and \blacklozenge) compared to 5 VJPs for the dense counterpart. With this simple example, we demonstrate a specific case where sparse reverse mode is more efficient than sparse forward mode and vice versa. `NonlinearSolve.jl` provides abstractions, allowing seamless switching between the modes for maximum performance. In [Subsection 3.4](#), we benchmark the scaling of sparse AD with regular AD on a steady-state PDE.

3. Special Capabilities. In the previous section, we provided an overview of solving nonlinear equations. Here, we will focus on specific capabilities of our package `NonlinearSolve.jl`. Let's cover the typical workflow of using `NonlinearSolve.jl`. First, we define the nonlinear equations. We will use a mutating function to compute our residual value from u and p and store it in F .

```
function f!(F, x, p)
    a, b, c = p
    F[1] = (x[1] + a) * (x[2]^3 - b) + c
    F[2] = sin(x[2]) * exp(x[1]) - 1
    return nothing
end
```

⁸For wider availability of the sparse Reverse Mode functionality, we make it available via `SparseDiffTools.jl` instead of `NonlinearSolve.jl`.

⁹We defer the discussion on the specifics of matrix coloring to [\[46\]](#).

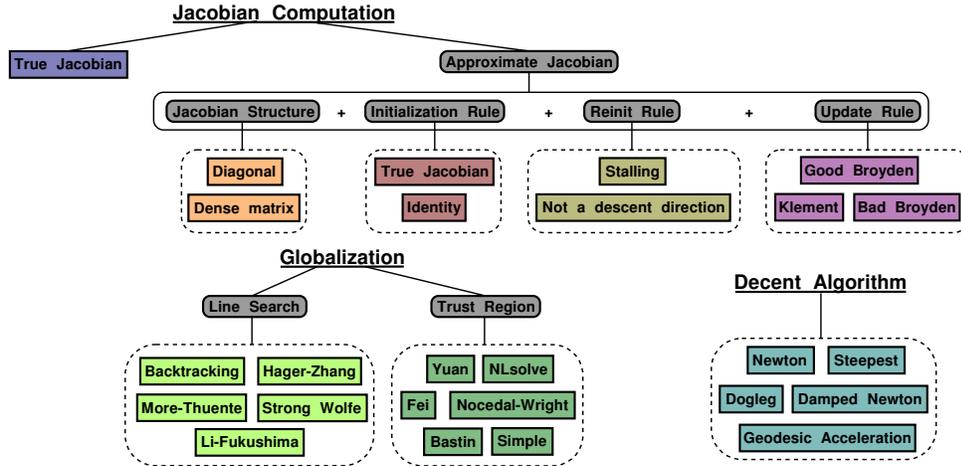


Fig. 3: `NonlinearSolve.jl` has a modular architecture with the core building blocks: Jacobian Computation Algorithm, Globalization Strategy, and Descent Algorithm. By combining these fundamental components, `NonlinearSolve.jl` facilitates creating diverse and powerful solver algorithms tailored to specific problem characteristics. This composability feature underscores the framework’s versatility in tackling a wide range of nonlinear equations, showcasing the potential for innovative algorithm development through the flexible integration of different strategies and techniques.

In Julia, mutating function names are appended with a `!` as a convention. Next, we construct a `NonlinearFunction` – a wrapper over `f!` that can store additional information like user-defined Jacobian functions and sparsity patterns.

```
nlfunc = NonlinearFunction(f!)
```

Next, we construct the `NonlinearProblem` with 2 arguments – the initial guess $u_0 = [0.0, 0.0]$, and the fixed parameters $p = [3.0, 7.0, 18.0]$.

```
prob = NonlinearProblem(nlfunc, [0.0, 0.0], [3.0, 7.0, 18.0])
```

Finally, calling `solve` on the problem uses a polyalgorithm [Subsection 3.2] to solve this problem. To use any other algorithm, we can pass it as the second argument.

```
solve(prob)
solve(prob, NewtonRaphson())
```

3.1. Composable Building Blocks. `NonlinearSolve.jl` stands out for its modular design, allowing users to combine various building blocks to create custom solver algorithms. This section delves into the flexibility and power of `NonlinearSolve.jl`’s architecture, focusing on its core components: Jacobian Computation Algorithm, Globalization Strategy, and Descent Algorithm.

1. Jacobian Computation: `NonlinearSolve.jl` supports a range of methods for Jacobian computation. Firstly, we support various automatic differentiation and finite differencing backends to compute the exact Jacobian. Additionally, to support Quasi-Newton methods, we provide different abstractions to iteratively approximate the Jacobian.
2. Globalization Strategy: This module facilitates the global convergence of the local solvers [Subsection 2.2] and can seamlessly integrate with the other

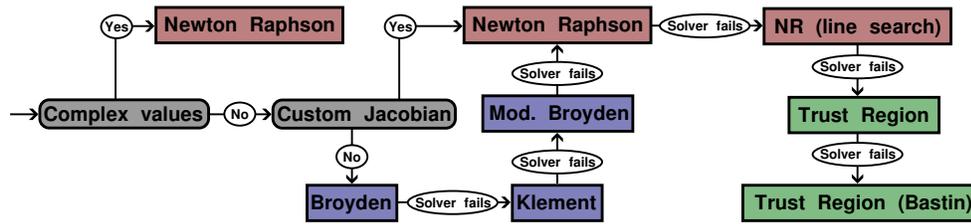


Fig. 4: **Default Nonlinear Solve PolyAlgorithm** focused on balancing speed and robustness. `NonlinearSolve.jl` first tries less robust Quasi-Newton methods for more performance and then tries more robust techniques if the faster ones fail.

blocks.

3. Descent Algorithm: These determine the direction vector given the Jacobian (or Higher-Order Derivatives) and the current value.

These building blocks provide a modular way to construct algorithms like:

Algorithm	Jacobian Strategy					Globalization	Descent
	True Jac.	Structure	Init. Rule	Reinit Rule	Update Rule		
NewtonRaphson	✓	-	-	-	-	-	Newton
NR (BackTracking)	✓	-	-	-	-	BackTracking	Newton
Trust Region	✓	-	-	-	-	Simple	Dogleg
TR (Bastin)	✓	-	-	-	-	Bastin	Dogleg
Broyden	✗	Dense	Identity	-	-	-	-
Limited Mem. Broyden	✗	Low Rank Matrix	Identity	Not a Des. Direction	Good Broyden	-	Newton
Mod. Broyden	✗	Dense	True Jac.	-	-	-	-
Klement	✗	Diagonal	Identity	Stalling	Klement	-	Newton
PseudoTransient	✓	-	-	-	-	-	DampedNewton
LevenbergMarquart	✓	-	-	-	-	Indirect TR Update	DampedNewton

The modular architecture of `NonlinearSolve.jl` not only supports a broad range of algorithms but also empowers users to craft sophisticated solver combinations. Among the possibilities, users can integrate Pseudo-Transient methods with Globalization strategies or pair Quasi-Newton Methods with Globalization techniques. This flexibility opens the door to creating tailored solutions that can more effectively navigate complex problem landscapes, highlighting `NonlinearSolve.jl`'s capability to adapt and optimize across a diverse set of nonlinear equation challenges.

3.2. Smart PolyAlgorithm Defaults. `NonlinearSolve.jl` comes with a set of well-benchmarked defaults designed to be fast and robust in the average case. For Nonlinear Problems with Intervals, we default to Interpolate, Truncate, and Project (ITP) [48]. For more advanced problems, we default to a polyalgorithm that selects the internal solvers based on the problem specification. Our selection happens two-fold, first at the nonlinear solver level [Figure 4] and next at the linear solver level¹⁰ [Figure 5].

3.2.1. Default Nonlinear Solver Selection. By default, we use a polyalgorithm that balances speed and robustness. We start with Quasi-Newton Algorithms – Broyden [49] and Klement [50]. If these fail, we use a modified version of Broyden,

¹⁰Default Linear Solver selection happens in `LinearSolve.jl`.

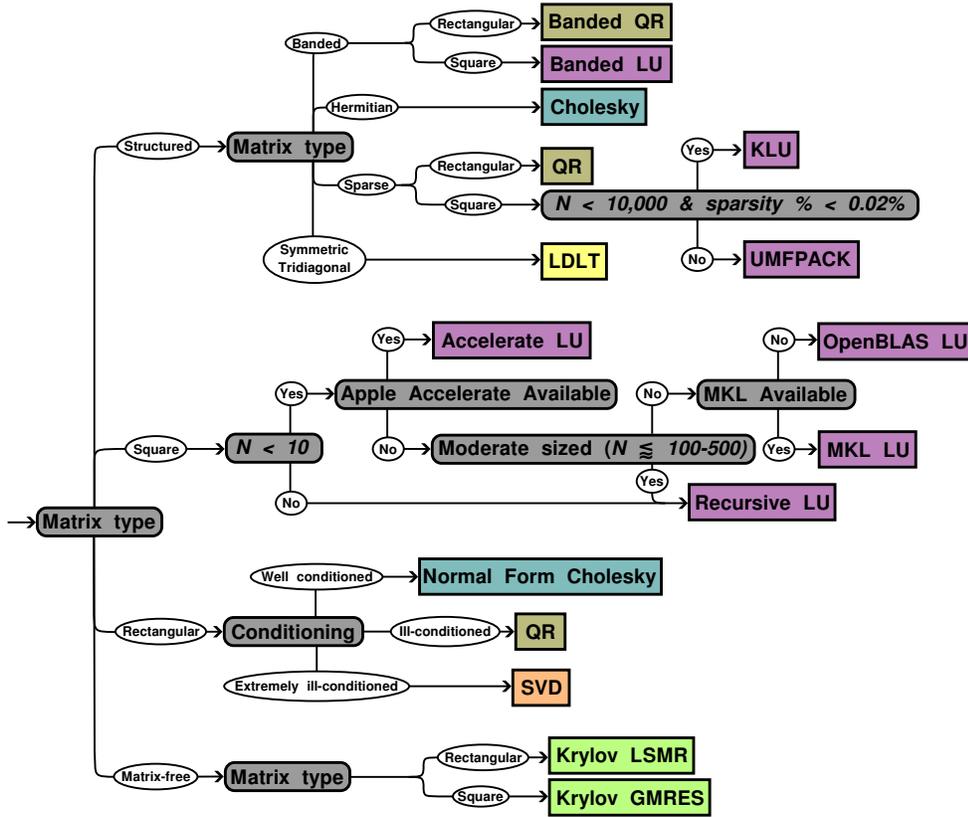


Fig. 5: **Decision Flowchart for Default Linear Solver Selection:** Starting with the determination of the Jacobian type (e.g., square, rectangular, symmetric, structured), the flowchart guides through various conditions such as sparsity and conditioning to select the most appropriate solver. Options range from specialized solvers like KLU for sparse matrices to robust methods like SVD for extremely ill-conditioned cases. This adaptive approach ensures that `NonlinearSolve.jl` utilizes the most efficient linear solver, enhancing performance and accuracy for a wide array of nonlinear problems

using a true Jacobian initialization. Finally, if Quasi-Newton Methods fail, we use Newton Raphson with Line Search and finally fall back to Trust Region Methods. Additionally, if a custom Jacobian function is provided or the system is small (≤ 25 states), we avoid using Quasi-Newton Methods and directly use the first-order solvers. We have designed our default to be robust, allowing it to solve all 23 test problems [Subsection 4.1]. Additionally, as seen in Figure 9, our default solver successfully solves new problems. Our default strongly contrasts with other software like `Sundials` and `MINPACK`, which can only solve 15 (22 with line search) and 17 (possibly 18, depending on settings) problems, respectively, out of the 23 problems.

3.2.2. Default Linear Solver Selection. For ill-conditioned Jacobians in the linear system ($Ax = b$), we default to QR for regular cases or SVD for extremely ill-conditioned cases. We run a polyalgorithm for well-conditioned systems to determine the best linear solver. If A is a matrix-free object, we use GMRES [51] from `Krylov.jl` [52] and solve the linear system without ever materializing the Jacobian.

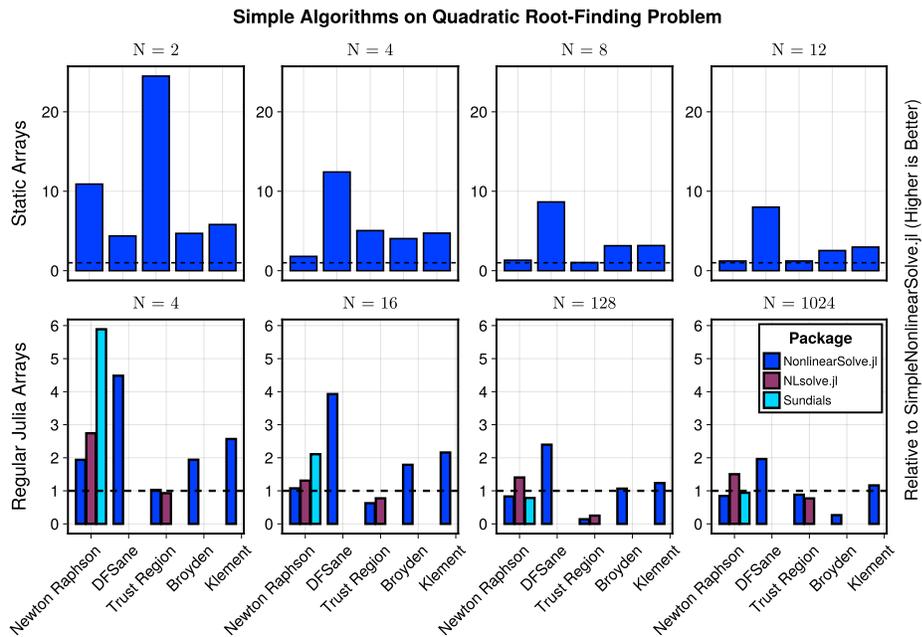


Fig. 6: `SimpleNonlinearSolve.jl` provides the fastest algorithms for `StaticArray` Problems, outperforming the same algorithms from `NonlinearSolve.jl` by a significant margin. For regular arrays, `SimpleNonlinearSolve.jl` is competitive to standard solvers up to a certain problem size threshold

For other cases, if A is reasonably small, we use the native Julia Implementation of LU Factorization [53] from `RecursiveFactorization.jl` [54]. We use the LU factorization routines from OpenBLAS or MKL for larger systems if present on the user’s system.

3.3. Non-Allocating Static Algorithms inside GPU Kernels. `NonlinearSolve.jl` comes bundled with `SimpleNonlinearSolve.jl`, which provides specialized non-allocating solvers for extremely efficient solving of very small nonlinear systems on GPUs. These solvers implement algorithms like `Newton-Raphson` and `Trust-Region` as static, non-allocating routines that operate directly on `StaticArrays` of fixed size, avoiding the overhead of allocations and dynamic dispatch. This makes them ideal for embedding inside GPU kernels using `KernelAbstractions.jl` [55] to solve many independent small nonlinear systems in parallel across GPU threads. In the following example, we solve the generalized Rosenbrock problem [Equation (2.12)] for 1024 different initial conditions on CPU, AMD ROCm GPUs and NVIDIA CUDA GPUs using the same code.

```

1 using NonlinearSolve, StaticArrays
2 using KernelAbstractions, CUDA, AMDGPU # For writing vendor-agnostic kernels
3
4 @kernel function parallel_nonlinearsolve_kernel!(result, @Const(prob), @Const(alg))
5     i = @index(Global)
6     prob_i = remake(prob; u0 = prob.u0[i])
7     sol = solve(prob_i, alg)
8     @inbounds result[i] = sol.u
9     return nothing
10 end
11
12 function vectorized_solve(prob, alg; backend = CPU())
13     result = KernelAbstractions.allocate(backend, eltype(prob.u0), length(prob.u0))
14

```

```

15  groupsize = min(length(prob.u0), 1024)
16
17  kernel! = parallel_nonlinearsolve_kernel!(backend, groupsize, length(prob.u0))
18  kernel!(result, prob, alg)
19  KernelAbstractions.synchronize(backend)
20
21  return result
22 end
23
24 @generated function generalized_rosenbrock(x::SVector{N}, p) where {N}
25  vals = ntuple(i -> gensym(string(i)), N)
26  expr = []
27  push!(expr, :($(vals[1]) = oneunit(x[1]) - x[1]))
28  for i in 2:N
29    push!(expr, :($(vals[i]) = 10.0 * (x[$i] - x[$i - 1]) * x[$i - 1]))
30  end
31  push!(expr, :(@SVector [$ (vals...) ]))
32  return Expr(:block, expr...)
33 end
34
35 u0 = @SVector [@SVector(rand(10)) for _ in 1:1024]
36 prob = NonlinearProblem(generalized_rosenbrock, u0)
37
38 # Threaded CPU
39 vectorized_solve(prob, SimpleNewtonRaphson(); backend = CPU())
40 # AMD ROCm GPU
41 vectorized_solve(prob, SimpleNewtonRaphson(); backend = ROCBackend())
42 # NVIDIA CUDA GPU
43 vectorized_solve(prob, SimpleNewtonRaphson(); backend = CUDABackend())

```

The simpler solvers outperform the more general solvers in `NonlinearSolve.jl` significantly for small static problems [Figure 6]. Their high performance enables applications like massively parallel global optimization [56] and parameter estimation problems, where solving many small independent nonlinear systems on the GPU is advantageous. `SimpleNonlinearSolve.jl` provides a portable, vendor-agnostic implementation that can target different GPU architectures like CUDA, ROCm, etc., with the same code.

3.4. Automatic Sparsity Exploitation. Symbolic sparsity detection has a high overhead for smaller systems with well-defined sparsity patterns. We provide an approximate algorithm to determine the Jacobian sparsity pattern in those setups. We compute the dense Jacobian for n randomly generated inputs to approximate the pattern. We take a union over the non-zero elements of Jacobian to obtain the Sparsity Pattern. As evident, computing the sparsity pattern costs n times the cost of computing the dense Jacobian, typically via automatic forward mode differentiation.

Approximate sparsity detection has poor scaling beyond a certain problem size, as evident from Figure 10. Similar to the shortcomings of other numerical sparsity detection software [43, 44], our method fails to accurately predict the sparsity pattern in the presence of state-dependent branches and might over-predict or under-predict sparsity due to floating point errors. Regardless, we observe in Figure 10 that approximate sparsity detection is extremely efficient for moderately sized problems. In addition to computing the Jacobian faster, sparsity detection enables us to sparse linear solvers that are significantly more efficient than solving the equivalent large dense linear systems [Subsection 4.3].

We rigorously benchmark the effects of sparsity detection algorithms in nonlinear root finding in Subsection 4.3. Here, we will isolate the cost of sparsity detection on a 2D Brusselator with increasing discretization. In Figure 7, we perform sparsity detection on the 2D Brusselator [Equation (4.1)] and compute the Jacobian 10 times to resemble a realistic workload where detection is performed once and reused for later iterations. We can see that a threaded implementation of forward mode AD (`PolyesterForwardDiff`) can compute the dense Jacobian faster than most sparse Jacobian algorithms for small problems. After an initial threshold, using approximate

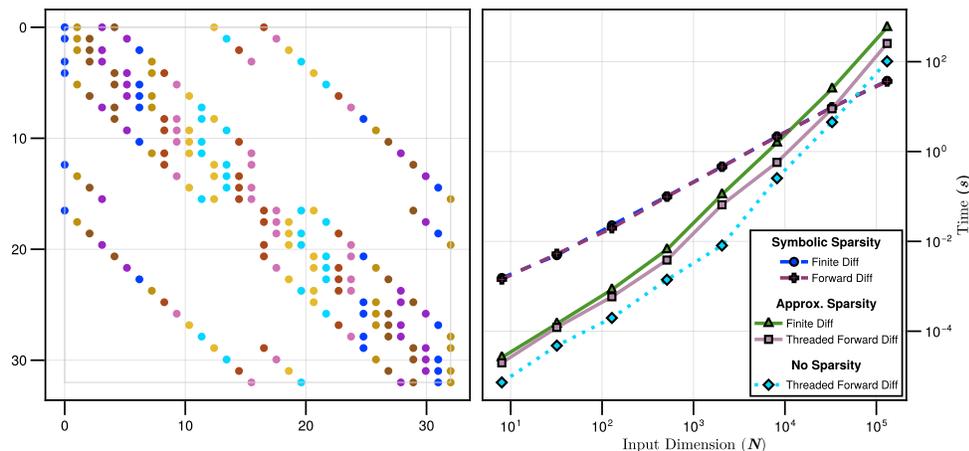


Fig. 7: **Automatic Sparsity Detection and Jacobian Computation for 2D Brusselator:** We benchmark the time taken to perform sparsity detection with automatic matrix coloring (left figure) and computing the Jacobian using the colored matrix. Sparsity detection has a high overhead for small systems, and threaded Forward Mode AD shines here. Threaded forward AD is always faster than approximate sparsity detection; however, in Figure 10, we show that detecting sparsity pattern enables the overall linear solve (and, in turn, the nonlinear solve) to be significantly faster. Additionally, we note that exact symbolic sparsity detection asymptotically leads to better scaling.

sparsity detection techniques will outperform other techniques. Finally, for large systems, using exact symbolic sparsity detection followed by colored AD is the most efficient.

3.5. Generalized Jacobian-Free Nonlinear Solvers using Krylov Methods.

`NonlinearSolve.jl` has built-in support for Jacobian-Free Solvers like Newton-Krylov, Dogleg with Krylov Methods, etc. We use the Iterative Linear Solvers from `LinearSolve.jl`. We use a `trait-based`¹¹ implementation to query if the provided linear solver can solve the system without materializing the matrix A . If the solver supports Matrix-Free linear solves, we construct a `JacobianOperator` which can compute $\mathcal{J}x$ using Forward Mode AD and $x^T \mathcal{J}$ using Reverse Mode AD. For example, consider the two most commonly used algorithms from `NonlinearSolve.jl` – `NewtonRaphson` and `TrustRegion`. `NewtonRaphson` computes the descent direction as:

$$(3.1) \quad \mathcal{J}_k \delta u_{\text{newton}} = -f(u_k, p)$$

Equation (3.1) can be trivially solved using Iterative Linear Solvers if we directly use Forward Mode AD to compute $\mathcal{J}_k \delta u_{\text{newton}}$. For Dogleg, we need δu_{newton} and δu_{sd} where:

$$(3.2) \quad \delta u_{\text{sd}} = -\mathcal{J}_k^T f(u_k, p)$$

We can compute δu_{sd} directly using Reverse Mode AD without computing \mathcal{J}_k . Additionally, providing a `JacobianOperator` that can compute both $x^T \mathcal{J}$ and $\mathcal{J}x$ enables

¹¹<https://invenia.github.io/blog/2019/11/06/julia-lang-features-part-2/>

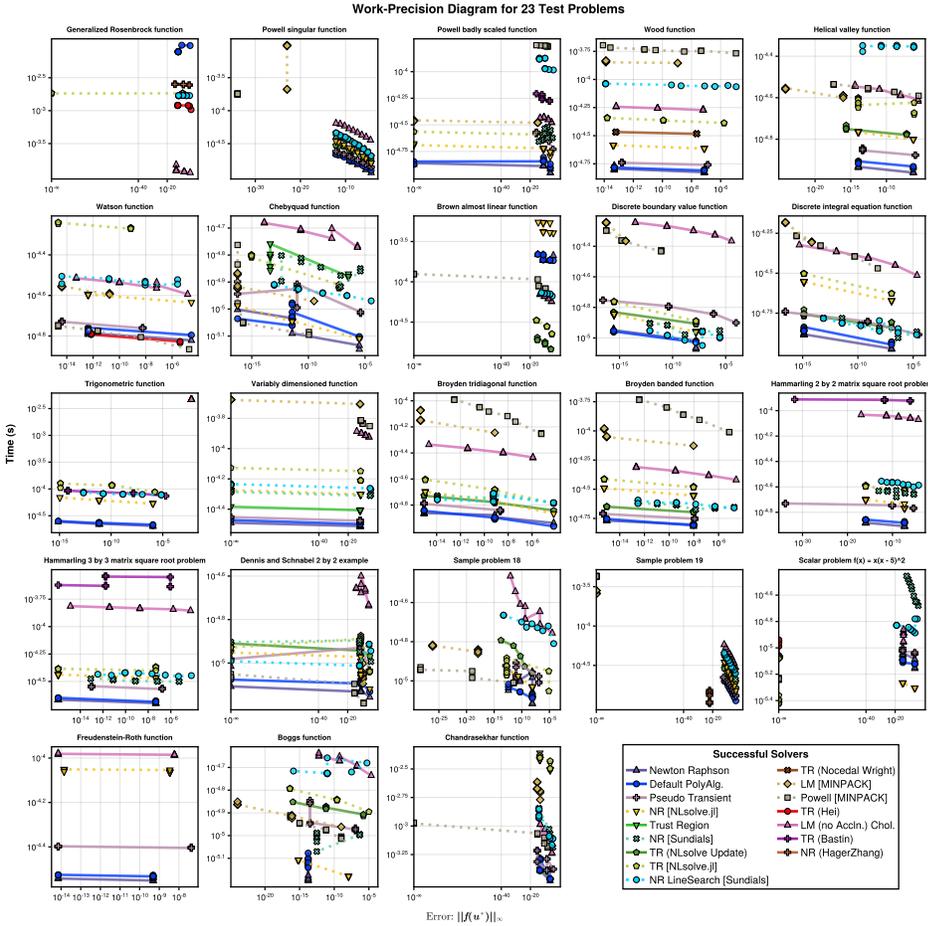


Fig. 8: **Work Precision Diagrams for 23 Test Problems:** Nonlinear-Solve.jl Solvers solve all of the 23 test problems. Our solvers perform runtime checks against various system parameters [Subsection 3.2] and dynamically select internal solvers to outperform other solvers like Sundials, MINPACK, and NLSolve.jl.

us to use Least Squares Krylov Methods like LSMR efficiently. For certain Krylov Methods to converge, it is imperative to use Linear Preconditioning, which often requires a materialized Jacobian. In such cases, we provide an external control – `concrete_jac` – that overrides the default choice between materialized Jacobian and `JacobianOperator` and forces a concrete materialized Jacobian if set to true. In Subsection 4.3, we demonstrate the use of Jacobian-Free Newton and Dogleg Methods with `GMRES` [51] and preconditioning from `IncompleteLU.jl` and `AlgebraicMultigrid.jl`. We show that for large-scale systems, Krylov Methods [Figure 11] significantly outperform other methods [Figure 10]. Additionally, all our sparse Jacobian tooling is compatible with the Krylov Solvers, allowing us to generate cheaper sparse Jacobians for the preconditioning.

4. Results. We evaluate our solvers on three numerical experiments and benchmark them against other nonlinear equation solvers – `NLSolve.jl` [20], `Sundi-`

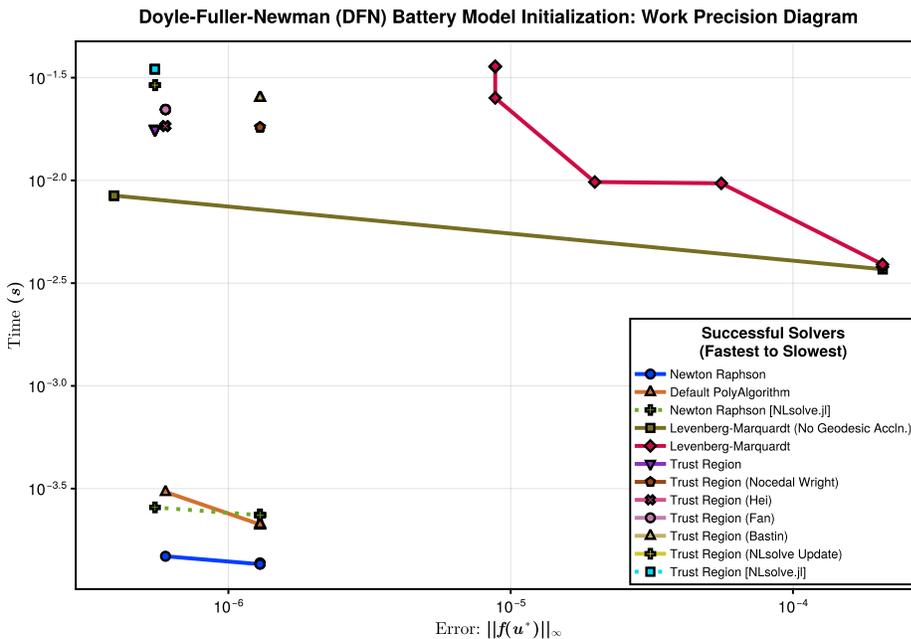


Fig. 9: **Initializing the Doyle-Fuller-Newman (DFN) Battery DAE Model at a High Current:** TrustRegion, NewtonRaphson, and LevenbergMarquardt from NonlinearSolve.jl reliably solve the DAE initialization problem and are faster than the corresponding NLSolve.jl equivalents. Sundials KINSOL and MINPACK fail to converge to the solution at any tolerance.

als [12, 13], and CMINPACK [15] (a modern C/C++ rewrite of MINPACK). We run all our benchmarks on Julia 1.10 on a cluster with 128 × AMD EPYC 7502 32-Core Processor with 128 Julia Threads. The code for our numerical experiments is publicly available on [GitHub](#)¹².

4.1. Robustness on 23 Test Problems. **23 Test Problems**¹³ is a suite of 23 small nonlinear systems, each with 1 – 10 variables, that provides a valuable resource for testing and evaluating nonlinear equation solvers. The problems cover various difficulties, making them suitable for various solver testing scenarios. The FORTRAN90 version of this test suite “includes routines defining the initial approximation to the solution of the system, the N function values at any point, and the N by N Jacobian matrix at any point.” We provide a pure Julia version of these problems in [NonlinearProblemLibrary.jl](#)¹⁴. In contrast to the FORTRAN90 version, we don’t implement the Jacobian functions and instead rely on the solvers using Automatic Differentiation or Finite Differencing to compute them.

For this experiment, we benchmark first-order solvers from various packages – Newton Raphson, Trust Region, and Levenberg Marquardt from NonlinearSolve.jl, Modified Powell and Levenberg Marquardt from CMINPACK, Newton Raphson, Trust Region and Anderson from NLSolve.jl, and Modified Newton Raphson from Sun-

¹²<https://github.com/SciML/SciMLBenchmarks.jl/tree/master/benchmarks/NonlinearProblem>

¹³https://people.sc.fsu.edu/~jburkardt/f_src/test_nonlin/test_nonlin.html

¹⁴<https://github.com/SciML/DiffEqProblemLibrary.jl/blob/master/lib/NonlinearProblemLibrary/src/NonlinearProblemLibrary.jl>

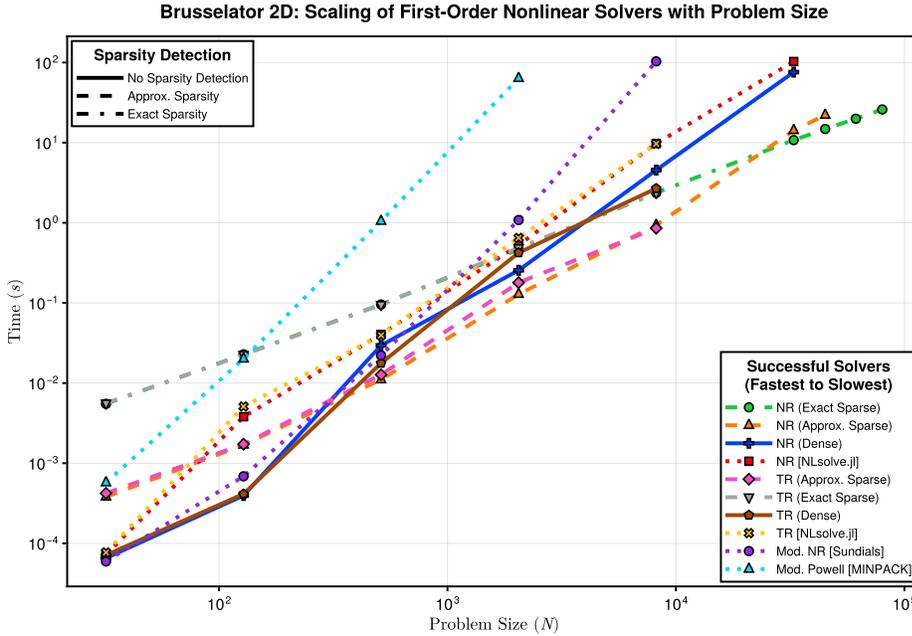


Fig. 10: **Brusselator 2D Scaling of First-Order Nonlinear Solvers:** `NonlinearSolve.jl` Newton-Raphson outperforms the implementation of the same algorithm from other frameworks. Notably, `NonlinearSolve.jl` is several orders of magnitude faster than MINPACK (written in C), which is widely used in software like SciPy and MATLAB. We show that `Approximate Sparsity Detection` accelerates moderately sized problems; however, at extremely large scale `Symbolic Sparsity Detection` outperforms all other methods by a margin.

dials KINSOL. For `NonlinearSolve.jl` native solvers, we perform additional analysis with different line search strategies – `HagerZhang`, `MoreThuente`, and `BackTracking` with `Newton Raphson`; different radius update schemes – `NLSolve`, `NocedalWright`, `Hei`, `Yuan`, `Bastin`, and `Fan` with `Trust Region`; and `Levenberg Marquardt` with and without `Geodesic Acceleration` [57]. Figure 8 shows that our solvers outperform other software packages.

4.2. Initializing the Doyle-Fuller-Newman (DFN) Battery Model. Initializing DAEs is a crucial step in the numerical solution process, as it ensures the consistency and well-posedness of the problem. Improper initialization can lead to convergence issues, inaccurate solutions, or even complete failure of the numerical solver. The initialization of DAEs involves determining consistent initial values for the differential and algebraic variables that satisfy the algebraic constraints at the initial time. This process is essential for ensuring that the numerical solution starts from a physically meaningful state and avoids violating the system constraints from the outset.

We generate a 32-dimensional DAE initialization problem for a `Doyle-Fuller-Newman (DFN) battery model`¹⁵ [58, 59] from open-circuit voltage (OCV) charged at a high current [60, 59]. We benchmark the following methods:

¹⁵<https://help.juliahub.com/batteries/stable/>

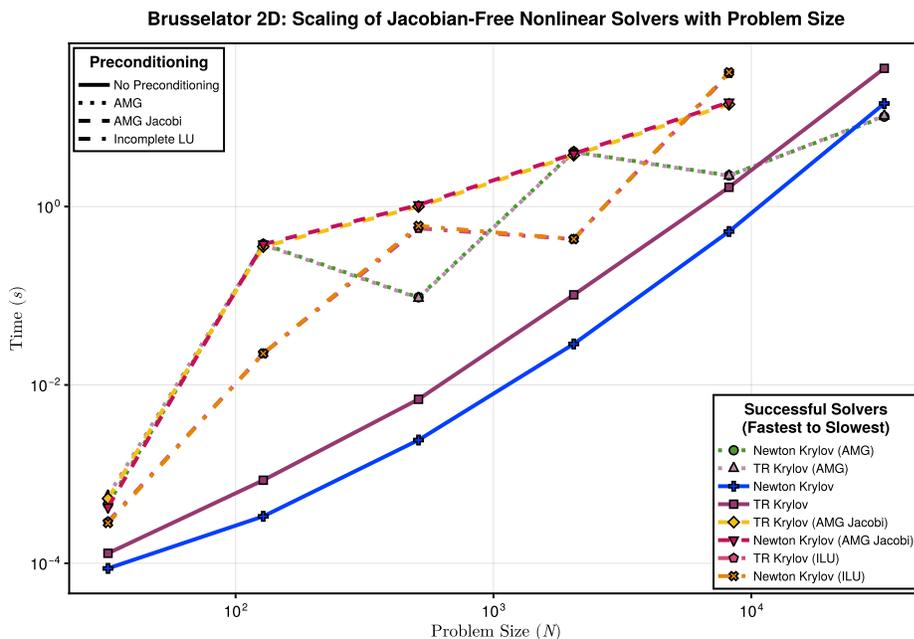


Fig. 11: **Brusselator 2D Scaling for Jacobian-Free Solvers:** `NonlinearSolve.jl` integrates with `LinearSolve.jl` to support Jacobian-Free Krylov Solvers, which can be set by passing `linsolve = KrylovJL_*` which can be `GMRES`, `CG`, `LSMR`, etc. to the solvers. Using Krylov Methods automatically prevents the Jacobian materialization, a major cost in Figure 10. Additionally, preconditioning the linear solve can help accelerate the overall root finding.

- TrustRegion from `NonlinearSolve.jl`, `NLSolve.jl`, and `MINPACK`.
- `NewtonRaphson` from `NonlinearSolve.jl`, `Sundials`, and `NLSolve.jl`.
- Quasi-Newton Methods from `NonlinearSolve.jl`.
- `LevenbergMarquardt` from `NonlinearSolve.jl` and `MINPACK`.

In Figure 9, we show that all the tested `NonlinearSolve.jl` solvers (except Quasi-Newton Methods¹⁶) solve the initialization problem. `Sundials` and `MINPACK` both are unable to solve the problem. `NLSolve.jl` successfully solves the problem, but their performance is consistently worse. Finally, we note that our polyalgorithm (without ever being tuned to this problem) successfully solves this problem.

4.3. Large Ill-Conditioned Nonlinear Brusselator System. Solving ill-conditioned nonlinear systems requires specializing the linear solver on properties of the Jacobian to cut down on the $O(n^3)$ linear solve and the $O(n^2)$ back-solves. We will use the sparsity detection and Jacobian-free solvers from `NonlinearSolve.jl` to solve the Steady State Stiff Brusselator PDE. The Brusselator PDE is defined as follows:

$$(4.1) \quad \begin{aligned} 0 &= 1 + u^2v - 4.4u + \alpha \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) + f(x, y, t) \\ 0 &= 3.4u - u^2v + \alpha \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right) \end{aligned}$$

¹⁶Quasi-Newton Methods are known to fail on this problem [60].

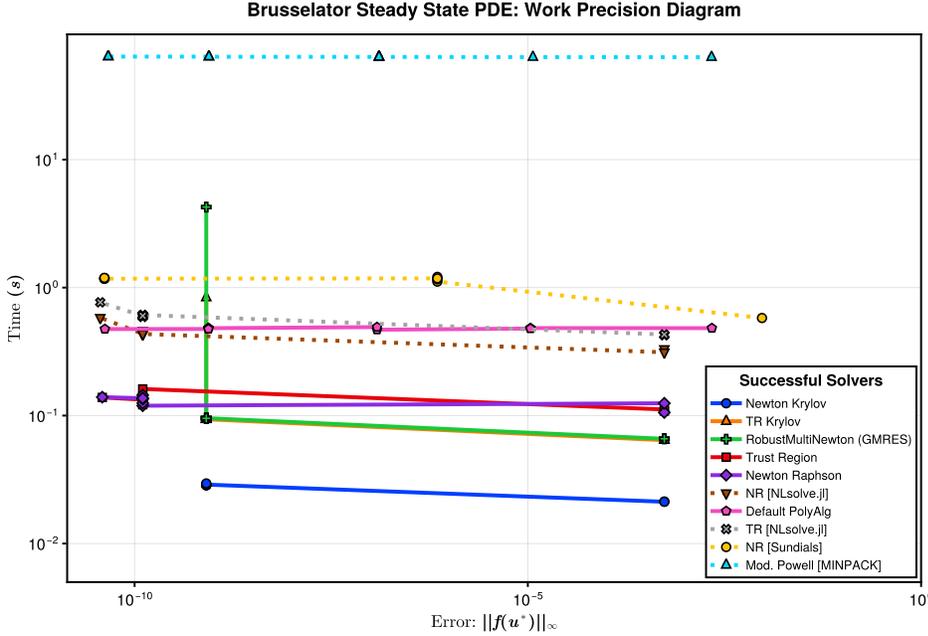


Fig. 12: **Work-Precision Diagram for Brusselator Steady State PDE:** `NewtonKrylov` from `NonlinearSolve.jl` is faster than the other solvers. `Sundials NewtonKrylov` could not solve the problem at any tolerance and was dropped from the plot.

where

$$(4.2) \quad f(x, y, t) = \begin{cases} 5 & \text{if } (x - 0.3)^2 + (y - 0.6)^2 \leq 0.1^2 \text{ and } t \geq 1.1 \\ 0 & \text{else} \end{cases}$$

and the initial conditions are

$$(4.3) \quad u(x, y, 0) = 22 \cdot (y(1 - y))^{3/2}$$

$$(4.4) \quad v(x, y, 0) = 27 \cdot (x(1 - x))^{3/2}$$

with the periodic boundary condition

$$(4.5) \quad u(x + 1, y, t) = u(x, y, t)$$

$$(4.6) \quad u(x, y + 1, t) = u(x, y, t)$$

We analyze our solvers for this problem in 3 parts. Firstly, [Figure 10](#) compares the scaling of `NewtonRaphson` and `TrustRegion` between frameworks. `NonlinearSolve.jl` leverages sparsity detection and colored sparse matrix algorithms to accelerate Jacobian construction and is consistently faster than all existing solvers here. None of the frameworks have built-in sparsity support and, unsurprisingly, don't scale well. However, with increasing discretization, explicitly forming Jacobians eventually becomes infeasible. [Figure 11](#) demonstrates `NonlinearSolve.jl` Jacobian-free Krylov Methods with Preconditioning that solve the linear system without constructing the Jacobian. We note that `Sundials KINSOL` with their built-in `GMRES` fails to converge to the solution, and `MINPACK` and `NLSolve.jl` don't support Jacobian-Free methods.

Finally, in [Figure 12](#), we present a Work-Precision Diagram for the discretized Brusselator on a 32×32 grid, showing that our methods are an order of magnitude faster than the ones in other software.

5. Conclusion. Solving systems of nonlinear equations is a fundamental challenge that arises across many scientific domains. This paper presented `NonlinearSolve.jl`, a high-performance and robust open-source solver for nonlinear systems implemented natively in the Julia programming language. Through extensive numerical experiments on benchmark problems, real-world applications, and scalability tests, we have demonstrated the superior capabilities of `NonlinearSolve.jl` compared to existing software tools.

Key strengths of `NonlinearSolve.jl` include its flexible unified API for rapidly experimenting with different solver options, smart automatic algorithm selection for balancing speed and robustness, specialized non-allocating kernels for small systems, automatic sparsity exploitation, and support for Jacobian-free Krylov methods. These features enable `NonlinearSolve.jl` to reliably solve challenging nonlinear problems, including cases where standard solvers fail while attaining high performance through techniques.

References.

- [1] Gerhard Wanner and Ernst Hairer. *Solving ordinary differential equations II*, volume 375. Springer Berlin Heidelberg New York, 1996.
- [2] Wayne H. Enright and Paul H. Muir. Runge-Kutta Software with Defect Control for Boundary Value ODEs. *SIAM J. Sci. Comput.*, 17:479–497, 1996.
- [3] Peter Deuffhard and Georg Bader. Multiple shooting techniques revisited. In *Numerical Treatment of Inverse Problems in Differential and Integral Equations: Proceedings of an International Workshop, Heidelberg, Fed. Rep. of Germany, August 30–September 3, 1982*, pages 74–94. Springer, 1983.
- [4] Uri M Ascher, Robert MM Mattheij, and Robert D Russell. *Numerical solution of boundary value problems for ordinary differential equations*. SIAM, 1995.
- [5] Weidong Zhang. Improved implementation of multiple shooting for BVPs. *Computer Science Department, University of Toronto*, 2012.
- [6] Shaojie Bai, J. Zico Kolter, and Vladlen Koltun. Deep Equilibrium Models. *arXiv:1909.01377 [cs, stat]*, October 2019. URL <http://arxiv.org/abs/1909.01377>. arXiv: 1909.01377.
- [7] Shaojie Bai, Vladlen Koltun, and J. Zico Kolter. Multiscale Deep Equilibrium Models. *arXiv:2006.08656 [cs, stat]*, November 2020. URL <http://arxiv.org/abs/2006.08656>. arXiv: 2006.08656.
- [8] Avik Pal, Alan Edelman, and Chris Rackauckas. Continuous Deep Equilibrium Models: Training Neural ODEs Faster by Integrating Them to Infinity. In *2023 IEEE High Performance Extreme Computing Conference (HPEC)*, pages 1–9, 2023. doi: 10.1109/HPEC58863.2023.10363574.
- [9] Avik Pal. On Efficient Training & Inference of Neural Differential Equations. Master’s thesis, Massachusetts Institute of Technology, 2023.
- [10] Jeff Bezanson, Alan Edelman, Stefan Karpinski, and Viral B Shah. Julia: A fresh approach to numerical computing. *SIAM review*, 59(1):65–98, 2017. URL <https://doi.org/10.1137/141000671>.
- [11] Yingbo Ma, Shashi Gowda, Ranjan Anantharaman, Chris Laughman, Viral Shah, and Chris Rackauckas. Modelingtoolkit: A composable graph transformation system for equation-based modeling, 2021.
- [12] David J Gardner, Daniel R Reynolds, Carol S Woodward, and Cody J Balos.

- Enabling new flexibility in the SUNDIALS suite of nonlinear and differential/algebraic equation solvers. *ACM Transactions on Mathematical Software (TOMS)*, 2022. doi: 10.1145/3539801.
- [13] Alan C Hindmarsh, Peter N Brown, Keith E Grant, Steven L Lee, Radu Serban, Dan E Shumaker, and Carol S Woodward. SUNDIALS: Suite of nonlinear and differential/algebraic equation solvers. *ACM Transactions on Mathematical Software (TOMS)*, 31(3):363–396, 2005. doi: 10.1145/1089014.1089020.
- [14] Jorge J Moré, Burton S Garbow, and Kenneth E Hillstom. User guide for MINPACK-1. Technical report, CM-P00068642, 1980.
- [15] Frédéric Devernay. C/C++ Minpack. <http://devernay.free.fr/hacks/cminpack/>, 2007.
- [16] Pauli Virtanen, Ralf Gommers, Travis E. Oliphant, Matt Haberland, Tyler Reddy, David Cournapeau, Evgeni Burovski, Pearu Peterson, Warren Weckesser, Jonathan Bright, Stéfan J. van der Walt, Matthew Brett, Joshua Wilson, K. Jarrod Millman, Nikolay Mayorov, Andrew R. J. Nelson, Eric Jones, Robert Kern, Eric Larson, C J Carey, İlhan Polat, Yu Feng, Eric W. Moore, Jake VanderPlas, Denis Laxalde, Josef Perktold, Robert Cimrman, Ian Henriksen, E. A. Quintero, Charles R. Harris, Anne M. Archibald, Antônio H. Ribeiro, Fabian Pedregosa, Paul van Mulbregt, and SciPy 1.0 Contributors. SciPy 1.0: Fundamental Algorithms for Scientific Computing in Python. *Nature Methods*, 17:261–272, 2020. doi: 10.1038/s41592-019-0686-2.
- [17] The MathWorks Inc. Optimization Toolbox version: 9.4 (R2022b), 2022. URL <https://www.mathworks.com>.
- [18] Satish Balay, Shrirang Abhyankar, Mark Adams, Jed Brown, Peter Brune, Kris Buschelman, Lisandro Dalcin, Alp Dener, Victor Eijkhout, W Gropp, et al. PETSc users manual. 2019.
- [19] Jason Rader, Terry Lyons, and Patrick Kidger. Optimistix: modular optimisation in JAX and Equinox. *arXiv preprint arXiv:2402.09983*, 2024.
- [20] Patrick Kofod Mogensen and Asbjørn Nilsen Riseth. Optim: A mathematical optimization package for Julia. *Journal of Open Source Software*, 3(24):615, 2018. doi: 10.21105/joss.00615.
- [21] Torkel E. Loman, Yingbo Ma, Vasily Ilin, Shashi Gowda, Niklas Korsbo, Nikhil Yewale, Chris Rackauckas, and Samuel A. Isaacson. Catalyst: Fast and flexible modeling of reaction networks. *PLOS Computational Biology*, 19(10):1–19, 10 2023. doi: 10.1371/journal.pcbi.1011530. URL <https://doi.org/10.1371/journal.pcbi.1011530>.
- [22] Bruno Cordani. *The Kepler Problem: Group Theoretical Aspects, Regularization and Quantization, with Application to the Study of Perturbations*, volume 29. Springer Science & Business Media, 2003.
- [23] Jorge Nocedal and Stephen J Wright. *Numerical optimization*. Springer, 1999.
- [24] F-A Potra and Vlastimil Pták. Nondiscrete induction and a double step secant method. *Mathematica Scandinavica*, 46(2):236–250, 1980.
- [25] Harmandeep Singh and Janak Raj Sharma. Simple yet highly efficient numerical techniques for systems of nonlinear equations. *Computational and Applied Mathematics*, 42(1):22, 2023.
- [26] Philip Wolfe. Convergence conditions for ascent methods. *SIAM review*, 11(2): 226–235, 1969.
- [27] Philip Wolfe. Convergence conditions for ascent methods. II: Some corrections. *SIAM review*, 13(2):185–188, 1971.
- [28] William W Hager and Hongchao Zhang. Algorithm 851: CG_DESCENT, a

- conjugate gradient method with guaranteed descent. *ACM Transactions on Mathematical Software (TOMS)*, 32(1):113–137, 2006.
- [29] Jorge J Moré and David J Thuente. Line search algorithms with guaranteed sufficient decrease. *ACM Transactions on Mathematical Software (TOMS)*, 20(3):286–307, 1994.
- [30] Long Hei. A self-adaptive trust region algorithm. *Journal of Computational Mathematics*, pages 229–236, 2003.
- [31] Ya-xiang Yuan. Recent advances in trust region algorithms. *Mathematical Programming*, 151:249–281, 2015.
- [32] Jinyan Fan. Convergence rate of the trust region method for nonlinear equations under local error bound condition. *Computational Optimization and Applications*, 34(2):215–227, 2006.
- [33] Fabian Bastin, Vincent Malmedy, Mélodie Mouffe, Philippe L Toint, and Dimitri Tomanos. A retrospective trust-region method for unconstrained optimization. *Mathematical programming*, 123:395–418, 2010.
- [34] Michael JD Powell. A hybrid method for nonlinear equations. *Numerical methods for nonlinear algebraic equations*, pages 87–161, 1970.
- [35] Avik Pal. Lux: Explicit parameterization of deep neural networks in julia. *GitHub repository*, 2022.
- [36] M Greta Ruppert, Yvonne Späck-Leigsnering, Julian Buschbaum, and Herbert De Gersem. Adjoint variable method for transient nonlinear electroquasistatic problems. *Electrical Engineering*, pages 1–7, 2023.
- [37] M Blondel, Q Berthet, M Cuturi, R Frostig, S Hoyer, and F Llinares-Lopez, f. pedregosa, and j.-p. vert, efficient and modular implicit differentiation. *arXiv preprint arXiv:2105.15183*, 2021.
- [38] Steven G Johnson. Notes on adjoint methods for 18.335. *Introduction to Numerical Methods*, 2006.
- [39] J. Revels, M. Lubin, and T. Papamarkou. Forward-Mode Automatic Differentiation in Julia. *arXiv:1607.07892 [cs.MS]*, 2016. URL <https://arxiv.org/abs/1607.07892>.
- [40] Michael Innes. Don’t Unroll Adjoint: Differentiating SSA-Form Programs. *CoRR*, abs/1810.07951, 2018. URL <http://arxiv.org/abs/1810.07951>.
- [41] Michael Innes, Elliot Saba, Keno Fischer, Dhairya Gandhi, Marco Concetto Rudilosso, Neethu Mariya Joy, Tejan Karmali, Avik Pal, and Viral Shah. Fashionable modelling with flux. *arXiv preprint arXiv:1811.01457*, 2018.
- [42] Brett M Averick, Jorge J Moré, Christian H Bischof, Alan Carle, and Andreas Griewank. Computing large sparse Jacobian matrices using automatic differentiation. *SIAM Journal on Scientific Computing*, 15(2):285–294, 1994.
- [43] Ralf Giering, Thomas Kaminski, and Thomas Slawig. Generating efficient derivative code with TAF: Adjoint and tangent linear Euler flow around an airfoil. *Future generation computer systems*, 21(8):1345–1355, 2005.
- [44] Andrea Walther and Andreas Griewank. Getting Started with ADOL-C. *Combinatorial scientific computing*, 181:202, 2009.
- [45] Shashi Gowda, Yingbo Ma, Valentin Churavy, Alan Edelman, and Christopher Rackauckas. Sparsity Programming: Automated Sparsity-Aware Optimizations in Differentiable Programming. In *Program Transformations for ML Workshop at NeurIPS 2019*, 2019.
- [46] Assefaw Hadish Gebremedhin, Fredrik Manne, and Alex Pothen. What color is your Jacobian? Graph coloring for computing derivatives. *SIAM review*, 47(4):629–705, 2005.

- [47] Pankaj Mishra, Shashi Gowda, Langwen Huang, and Chris Rackauckas. SparseDiffTools.jl. JuliaDiff/SparseDiffTools.jl, 2020.
- [48] Ivo FD Oliveira and Ricardo HC Takahashi. An enhancement of the bisection method average performance preserving minmax optimality. *ACM Transactions on Mathematical Software (TOMS)*, 47(1):1–24, 2020.
- [49] Charles G Broyden. A class of methods for solving nonlinear simultaneous equations. *Mathematics of computation*, 19(92):577–593, 1965.
- [50] Jan Klement. On using quasi-newton algorithms of the Broyden class for model-to-test correlation. *Journal of Aerospace Technology and Management*, 6:407–414, 2014.
- [51] Youcef Saad and Martin H Schultz. GMRES: A generalized minimal residual algorithm for solving nonsymmetric linear systems. *SIAM Journal on scientific and statistical computing*, 7(3):856–869, 1986.
- [52] Alexis Montoisson and Dominique Orban. Krylov.jl: A Julia basket of hand-picked Krylov methods. *Journal of Open Source Software*, 8(89):5187, 2023. doi: 10.21105/joss.05187.
- [53] Sivan Toledo. Locality of reference in LU decomposition with partial pivoting. *SIAM Journal on Matrix Analysis and Applications*, 18(4):1065–1081, 1997.
- [54] Yingbo Ma and Chris Elrod. GitHub - JuliaLinearAlgebra/RecursiveFactorization.jl — github.com. <https://github.com/JuliaLinearAlgebra/RecursiveFactorization.jl>. [Accessed 16-02-2024].
- [55] V Churavy, D Aluthge, LC Wilcox, S Byrne, M Waruszewski, A Ramadhan, S Schaub Meredith, J Schloss, J Samaroo, J Bolewski, et al. JuliaGPU/KernelAbstractions.jl: v0. 6.0, 2021.
- [56] Utkarsh, Vaibhav Kumar Dixit, Julian Samaroo, Avik Pal, Alan Edelman, and Christopher Vincent Rackauckas. Efficient GPU-Accelerated Global Optimization for Inverse Problems. In *ICLR 2024 Workshop on AI4DifferentialEquations In Science*, 2024. URL <https://openreview.net/forum?id=nD10o1ge97>.
- [57] Mark K Transtrum and James P Sethna. Improvements to the Levenberg-Marquardt algorithm for nonlinear least-squares minimization. *arXiv preprint arXiv:1201.5885*, 2012.
- [58] Marc Doyle, Thomas F Fuller, and John Newman. Modeling of galvanostatic charge and discharge of the lithium/polymer/insertion cell. *Journal of the Electrochemical society*, 140(6):1526, 1993.
- [59] Chris Rackauckas, Maja Gwozdz, Anand Jain, Yingbo Ma, Francesco Martinuzzi, Utkarsh Rajput, Elliot Saba, Viral B Shah, Ranjan Anantharaman, Alan Edelman, et al. Composing modeling and simulation with machine learning in julia. In *2022 Annual Modeling and Simulation Conference (ANNSIM)*, pages 1–17. IEEE, 2022.
- [60] Marc D Berliner, Daniel A Cogswell, Martin Z Bazant, and Richard D Braatz. Methods—PETLION: Open-source software for millisecond-scale porous electrode theory-based lithium-ion battery simulations. *Journal of The Electrochemical Society*, 168(9):090504, 2021.