

ROBER Work-Precision Diagrams

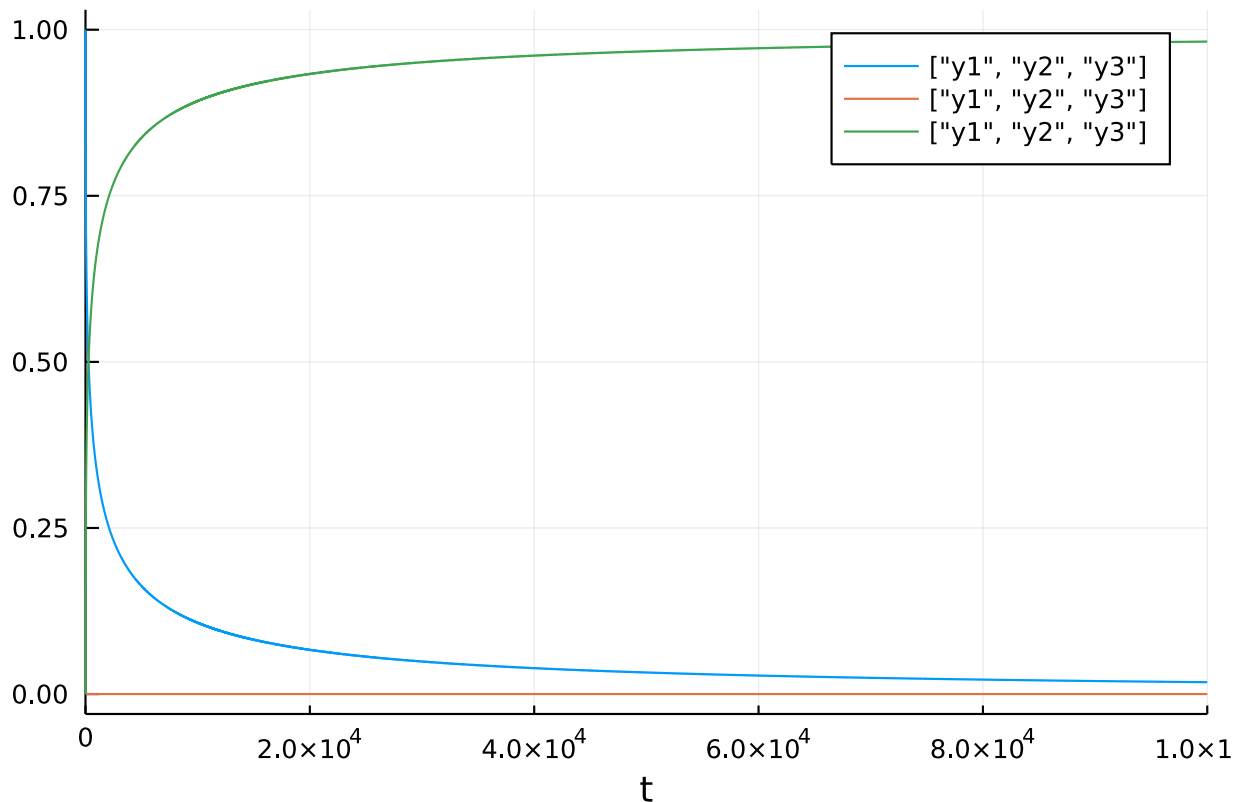
Chris Rackauckas

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```
using OrdinaryDiffEq, DiffEqDevTools, Sundials, ParameterizedFunctions, Plots, ODE,
ODEInterfaceDiffEq, LSODA
gr()
using LinearAlgebra

rober = @ode_def begin
    dy_1 = -k_1*y_1+k_3*y_2*y_3
    dy_2 = k_1*y_1-k_2*y_2^2-k_3*y_2*y_3
    dy_3 = k_2*y_2^2
end k_1 k_2 k_3
prob = ODEProblem(rober, [1.0, 0.0, 0.0], (0.0, 1e5), (0.04, 3e7, 1e4))
sol = solve(prob, CVODE_BDF(), abstol=1/10^14, reltol=1/10^14)
test_sol = TestSolution(sol)
abstols = 1.0 ./ 10.0 .^ (4:11)
reltols = 1.0 ./ 10.0 .^ (1:8);

plot(sol, labels=["y1", "y2", "y3"])
```



0.1 Omissions And Tweaking

The following were omitted from the tests due to convergence failures. ODE.jl's adaptivity is not able to stabilize its algorithms, while GeometricIntegratorsDiffEq has not upgraded to Julia 1.0. GeometricIntegrators.jl's methods used to be either fail to converge at comparable dts (or on some computers errors due to type conversions).

```
#sol = solve(prob,ode23s()); println("Total ODE.jl steps: $(length(sol))")
#using GeometricIntegratorsDiffEq
#try
#    sol = solve(prob,GIRadIIA3(),dt=1/10)
#catch e
#    println(e)
#end
```

ARKODE needs a lower `nonlinear_convergence_coefficient` in order to not diverge.

```
#sol = solve(prob,ARKODE(nonlinear_convergence_coefficient =
1e-6), abstol=1e-5, reltol=1e-1); # Noisy, output omitted
```

```
sol = solve(prob,ARKODE(nonlinear_convergence_coefficient =
1e-7), abstol=1e-5, reltol=1e-1);
```

Note that `1e-7` matches the value from the Sundials manual which was required for their example to converge on this problem. The default is `1e-1`.

```
#sol = solve(prob,ARKODE(order=3), abstol=1e-4, reltol=1e-1); # Fails to diverge but
doesn't finish
```

```
#sol = solve(prob,ARKODE(order=5), abstol=1e-4, reltol=1e-1); # Noisy, output omitted
```

```
#sol = solve(prob,ARKODE(order=5, nonlinear_convergence_coefficient =
1e-9), abstol=1e-5, reltol=1e-1); # Noisy, output omitted
```

Additionally, the ROCK methods do not perform well on this benchmark.

```
setups = [
    #Dict(:alg=>ROCK2())      #Unstable
    #Dict(:alg=>ROCK4())      #needs more iterations
]
```

Any[]

Some of the bad Rosenbrocks fail:

```
setups = [
    #Dict(:alg=>Hairer4()),
    #Dict(:alg=>Hairer42()),
    #Dict(:alg=>Cash4()),
]
```

Any[]

The EPIRK and exponential methods also fail:

```
sol = solve(prob,EXPRB53s3(),dt=2.0^(-8));
sol = solve(prob,EPIRK4s3B(),dt=2.0^(-8));
sol = solve(prob,EPIRK5P2(),dt=2.0^(-8));
```

Error: InexactError: trunc{Int64, Inf}

PDIRK44 also fails

```
sol = solve(prob,PDIRK44(),dt=2.0^(-8));
```

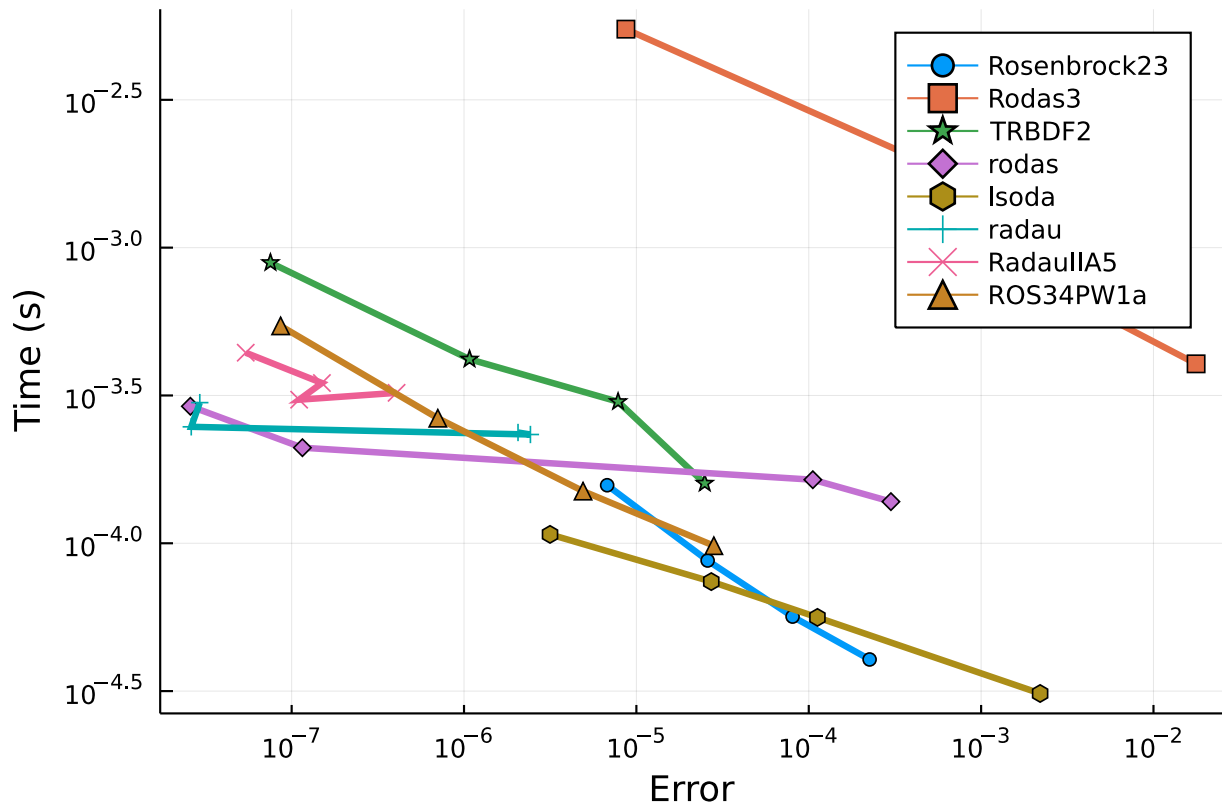
In fact, all non-adaptive methods fail on this problem.

0.2 High Tolerances

This is the speed when you just want the answer. `ode23s` from `ODE.jl` was removed since it fails. Note that at high tolerances Sundials' `CVODE_BDF` fails as well so it's excluded from this test.

```
abstols = 1.0 ./ 10.0 .^ (5:8)
reltols = 1.0 ./ 10.0 .^ (1:4);
setup = [Dict(:alg=>Rosenbrock23()),
         Dict(:alg=>Rodas3()),
         Dict(:alg=>TRBDF2()),
         Dict(:alg=>rodas()),
         Dict(:alg=>lsoda()),
         Dict(:alg=>radau()),
         Dict(:alg=>RadauIIA5()),
         Dict(:alg=>ROS34PW1a()),
       ]

gr()
wp = WorkPrecisionSet(prob,abstols,reltols,setup;
                      save_everystep=false,appxsol=test_sol,maxiters=Int(1e5),numruns=10)
plot(wp)
```

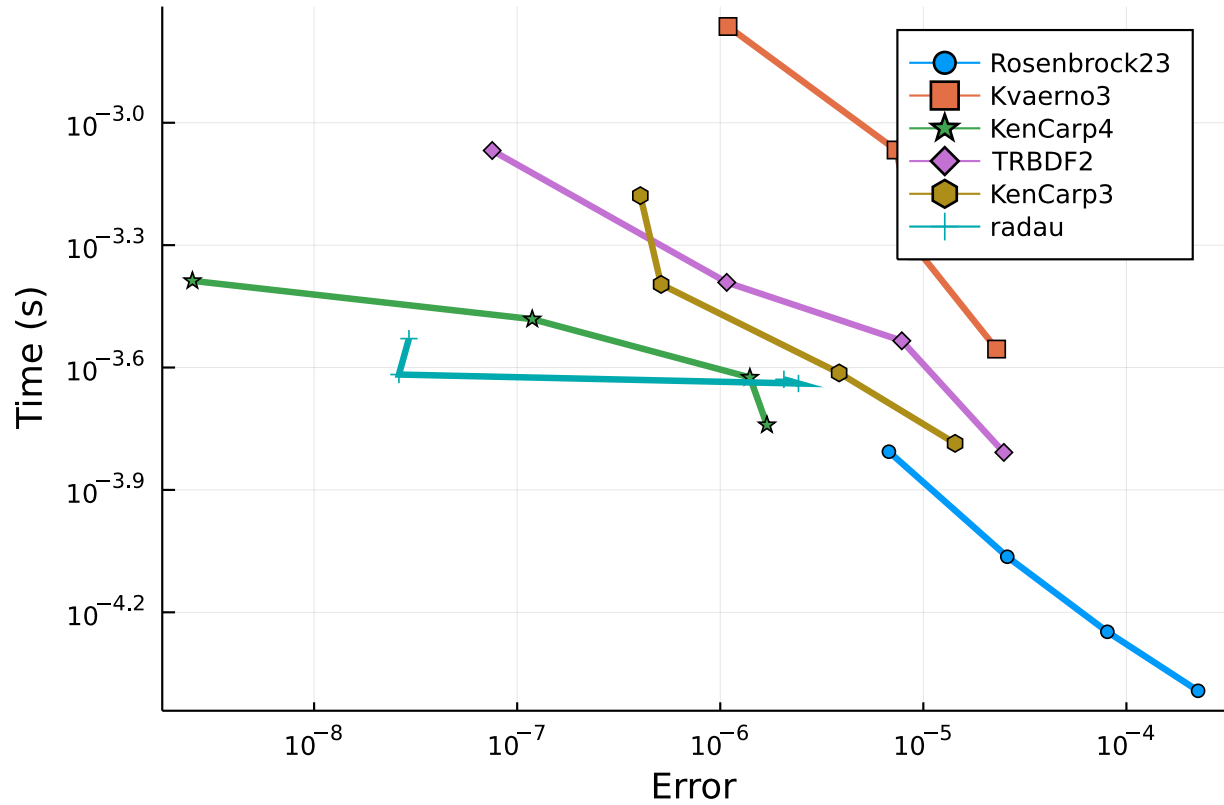


```
setup = [Dict(:alg=>Rosenbrock23()),
         Dict(:alg=>Kvaerno3()),
         Dict(:alg=>KenCarp4()),
```

```

Dict(:alg=>TRBDF2()),
Dict(:alg=>KenCarp3()),
# Dict(:alg=>SDIRK2()), # Removed because it's bad
Dict(:alg=>radau())
names = ["Rosenbrock23" "Kvaerno3" "KenCarp4" "TRBDF2" "KenCarp3" "radau"]
wp = WorkPrecisionSet(prob, abstols, reltols, setups; names=names,
    save_everystep=false, appxsol=test_sol, maxiters=Int(1e5), numruns=10)
plot(wp)

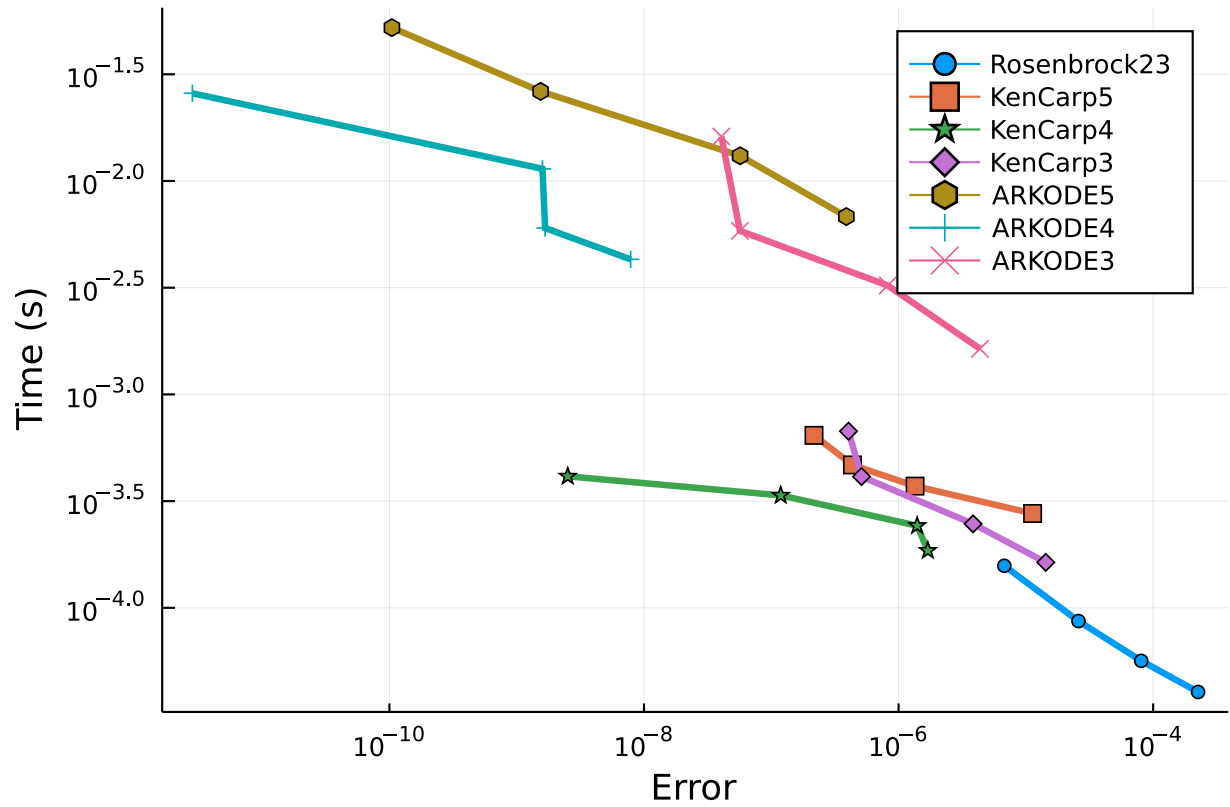
```



```

setups = [Dict(:alg=>Rosenbrock23()),
    Dict(:alg=>KenCarp5()),
    Dict(:alg=>KenCarp4()),
    Dict(:alg=>KenCarp3()),
    Dict(:alg=>ARKODE(nonlinear_convergence_coefficient = 1e-9, order=5)),
    Dict(:alg=>ARKODE(nonlinear_convergence_coefficient = 1e-8)),
    Dict(:alg=>ARKODE(nonlinear_convergence_coefficient = 1e-7, order=3))
]
names = ["Rosenbrock23" "KenCarp5" "KenCarp4" "KenCarp3" "ARKODE5" "ARKODE4" "ARKODE3"]
wp = WorkPrecisionSet(prob, abstols, reltols, setups;
    names=names,
    save_everystep=false, appxsol=test_sol, maxiters=Int(1e5), numruns=10)
plot(wp)

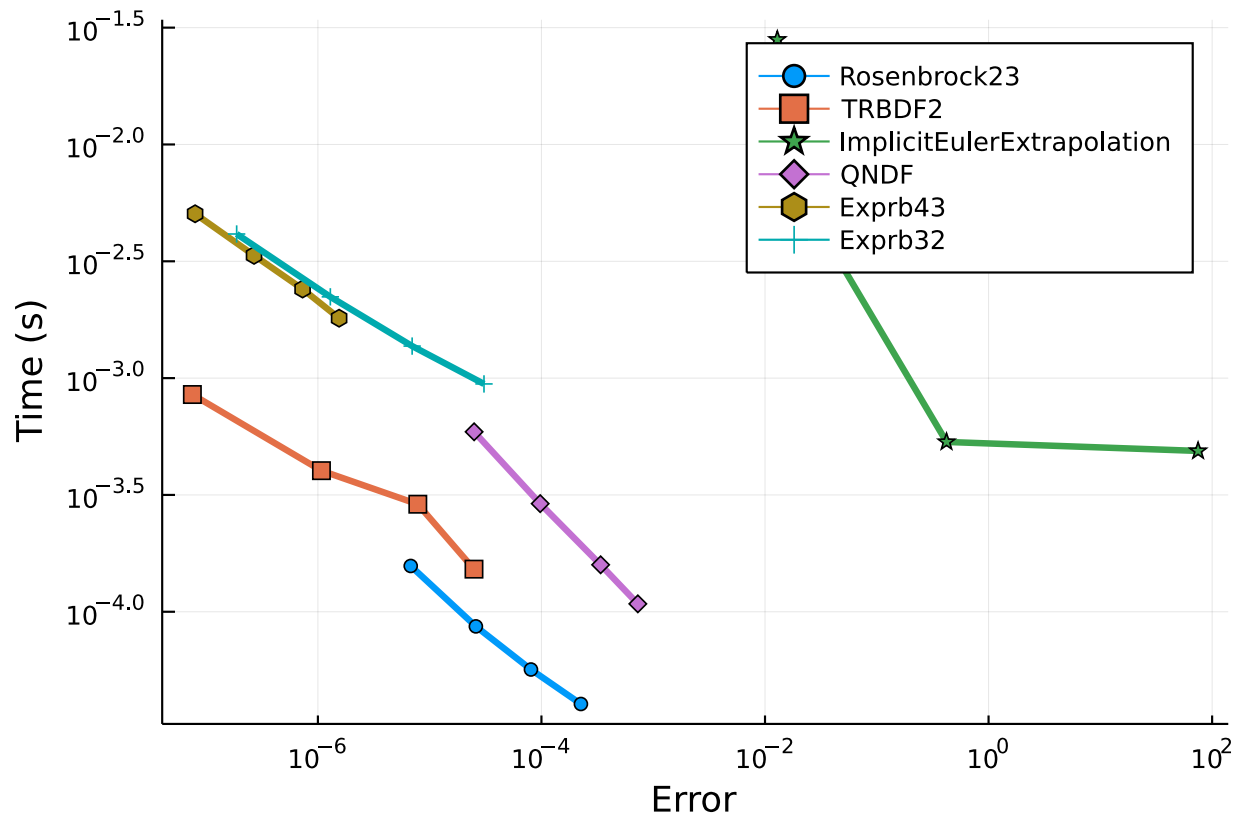
```



```

setups = [Dict(:alg=>Rosenbrock23()),
           Dict(:alg=>TRBDF2()),
           Dict(:alg=>ImplicitEulerExtrapolation()),
           #Dict(:alg=>ImplicitDeuflhardExtrapolation()), # Diverges
           #Dict(:alg=>ImplicitHairerWannerExtrapolation()), # Diverges
           #Dict(:alg=>ABDF2()), # Maxiters
           Dict(:alg=>QNDF()),
           Dict(:alg=>Exprb43()),
           Dict(:alg=>Exprb32()),
        ]
wp = WorkPrecisionSet(prob, abstols, reltols, setups;
                      save_everystep=false, appxsol=test_sol, maxiters=Int(1e5), numruns=10)
plot(wp)

```



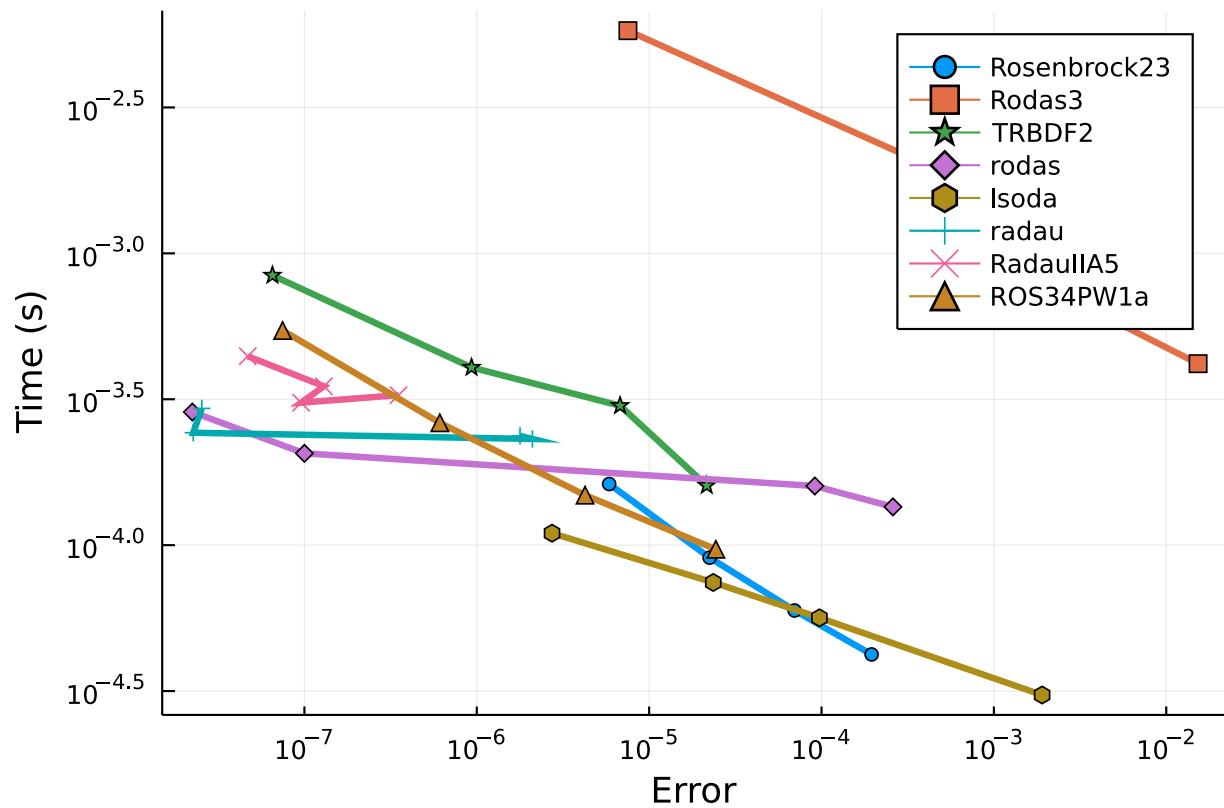
0.2.1 Timeseries Errors

```

abstols = 1.0 ./ 10.0 .^ (5:8)
reltols = 1.0 ./ 10.0 .^ (1:4);
setup = [Dict(:alg=>Rosenbrock23()),
         Dict(:alg=>Rodas3()),
         Dict(:alg=>TRBDF2()),
         Dict(:alg=>rodas()),
         Dict(:alg=>lsoda()),
         Dict(:alg=>radau()),
         Dict(:alg=>RadauIIA5()),
         Dict(:alg=>ROS34PW1a()),
         ]

gr()
wp = WorkPrecisionSet(prob,abstols,reltols,setup;error_estimate=:l2,
                     save_everystep=false,appxsol=test_sol,maxiters=Int(1e5),numruns=10)
plot(wp)

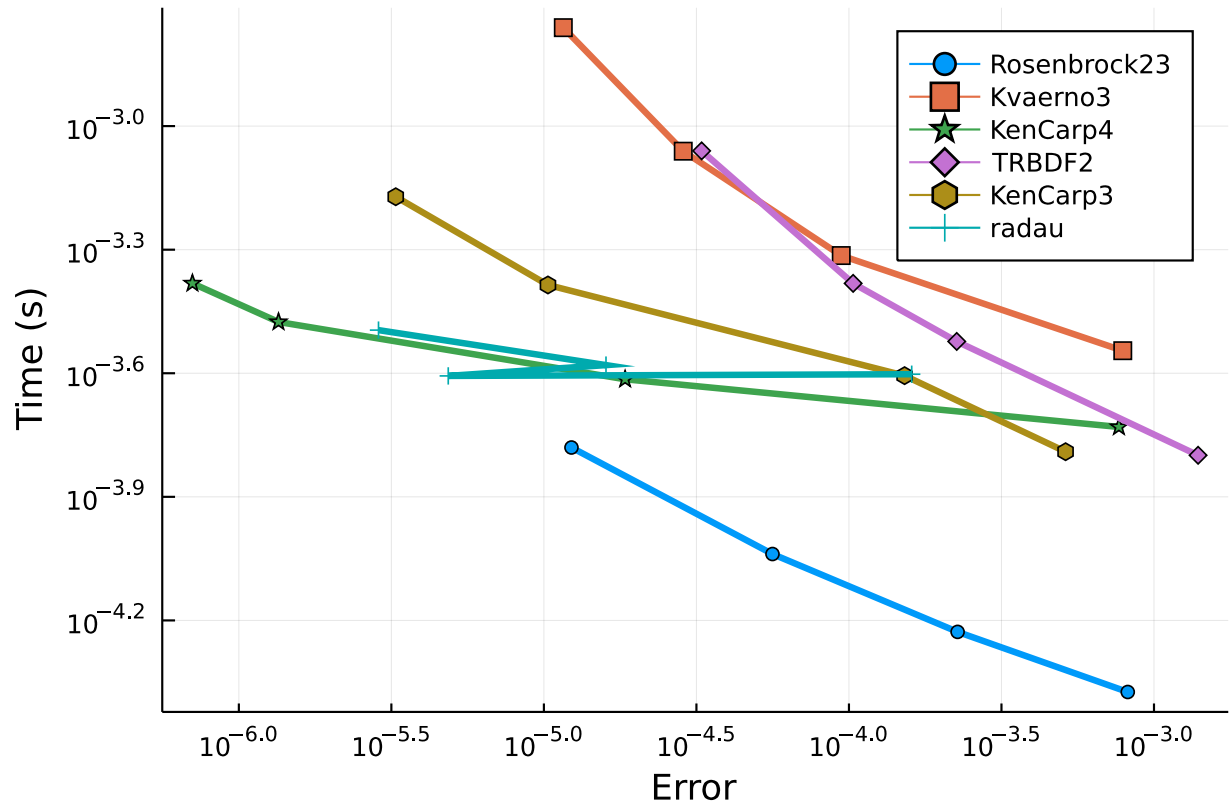
```



```

setups = [Dict(:alg=>Rosenbrock23()),
          Dict(:alg=>Kvaerno3()),
          Dict(:alg=>KenCarp4()),
          Dict(:alg=>TRBDF2()),
          Dict(:alg=>KenCarp3()),
          # Dict(:alg=>SDIRK2()), # Removed because it's bad
          Dict(:alg=>radau())]
names = ["Rosenbrock23" "Kvaerno3" "KenCarp4" "TRBDF2" "KenCarp3" "radau"]
wp = WorkPrecisionSet(prob, abstols, reltols, setups; names=names,
                      appxsol=test_sol, maxiters=Int(1e5), error_estimate=:l2, numruns=10)
plot(wp)

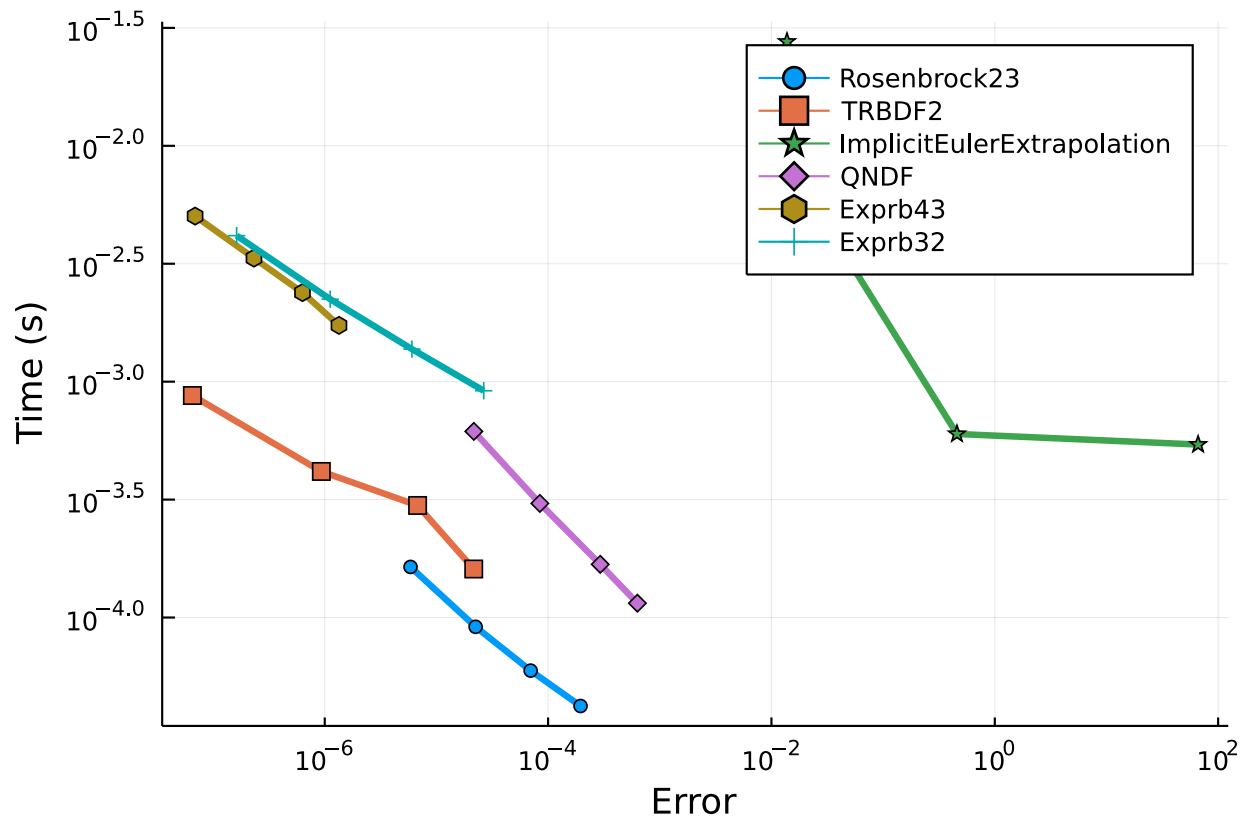
```



```

setups = [Dict(:alg=>Rosenbrock23()),
          Dict(:alg=>TRBDF2()),
          Dict(:alg=>ImplicitEulerExtrapolation()),
          #Dict(:alg=>ImplicitDeuflhardExtrapolation()), # Diverges
          #Dict(:alg=>ImplicitHairerWannerExtrapolation()), # Diverges
          #Dict(:alg=>ABDF2()), # Maxiters
          Dict(:alg=>QNDF()),
          Dict(:alg=>Exprb43()),
          Dict(:alg=>Exprb32()),
        ]
wp = WorkPrecisionSet(prob, abstols, reltols, setups; verbose=false, error_estimate=:l2,
                     save_everystep=false, appxsol=test_sol, maxiters=Int(1e5), numruns=10)
plot(wp)

```

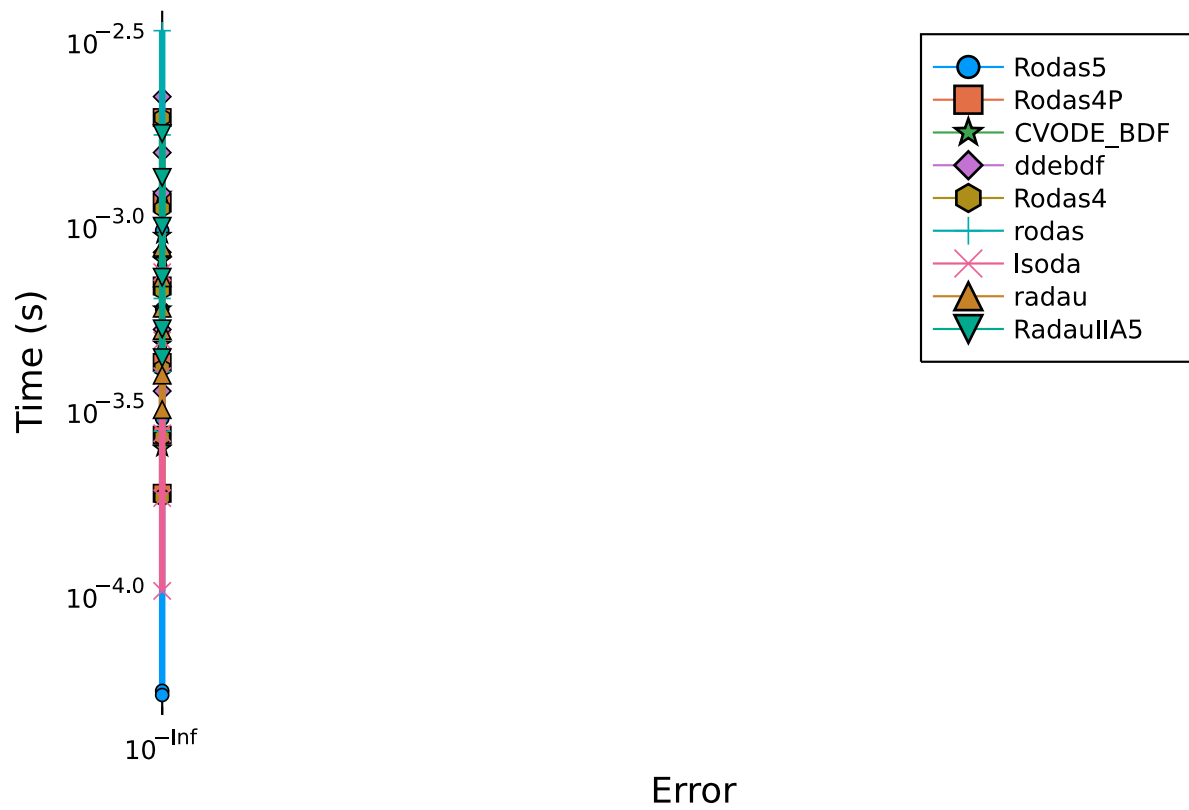



0.2.2 Low Tolerances

This is the speed at lower tolerances, measuring what's good when accuracy is needed.

```
abstols = 1.0 ./ 10.0 .^ (7:12)
reltols = 1.0 ./ 10.0 .^ (4:9)
```

```
setups = [Dict(:alg=>Rodas5()),
          Dict(:alg=>Rodas4P()),
          Dict(:alg=>CVODE_BDF()),
          Dict(:alg=>ddebdf()),
          Dict(:alg=>Rodas4()),
          Dict(:alg=>rodas()),
          Dict(:alg=>lsoda()),
          Dict(:alg=>radau()),
          Dict(:alg=>RadauIIA5()),
        ]
wp = WorkPrecisionSet(prob,abstols,reltols,setups;
                     save_everystep=false,appxsol=test_sol,maxiters=Int(1e5),numruns=10)
plot(wp)
```



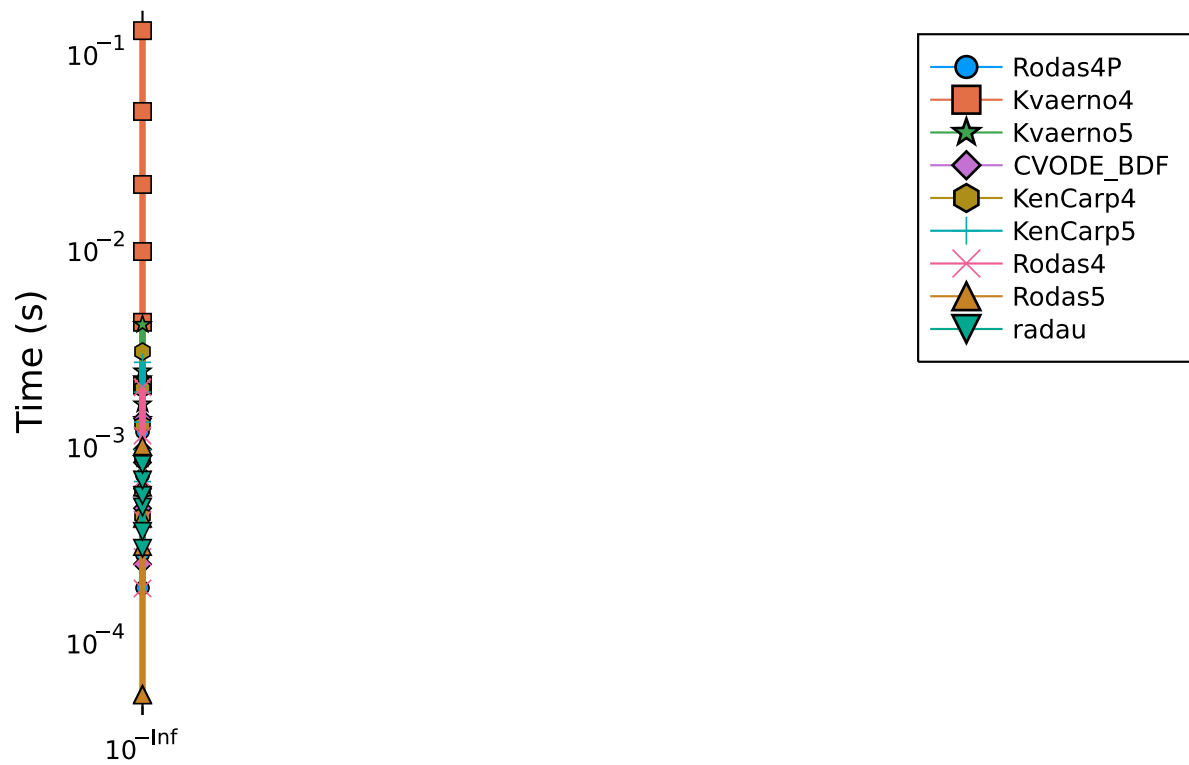
```

setups = [Dict(:alg=>Rodas4P()),
          Dict(:alg=>Kvaerno4()),
          Dict(:alg=>Kvaerno5()),
          Dict(:alg=>CVODE_BDF()),
          Dict(:alg=>KenCarp4()),
          Dict(:alg=>KenCarp5()),
          Dict(:alg=>Rodas4()),
          Dict(:alg=>Rodas5()),
          Dict(:alg=>radau())]

wp = WorkPrecisionSet(prob, abstols, reltols, setups;
                     save_everystep=false, appxsol=test_sol, maxiters=Int(1e5), numruns=10)

plot(wp)

```

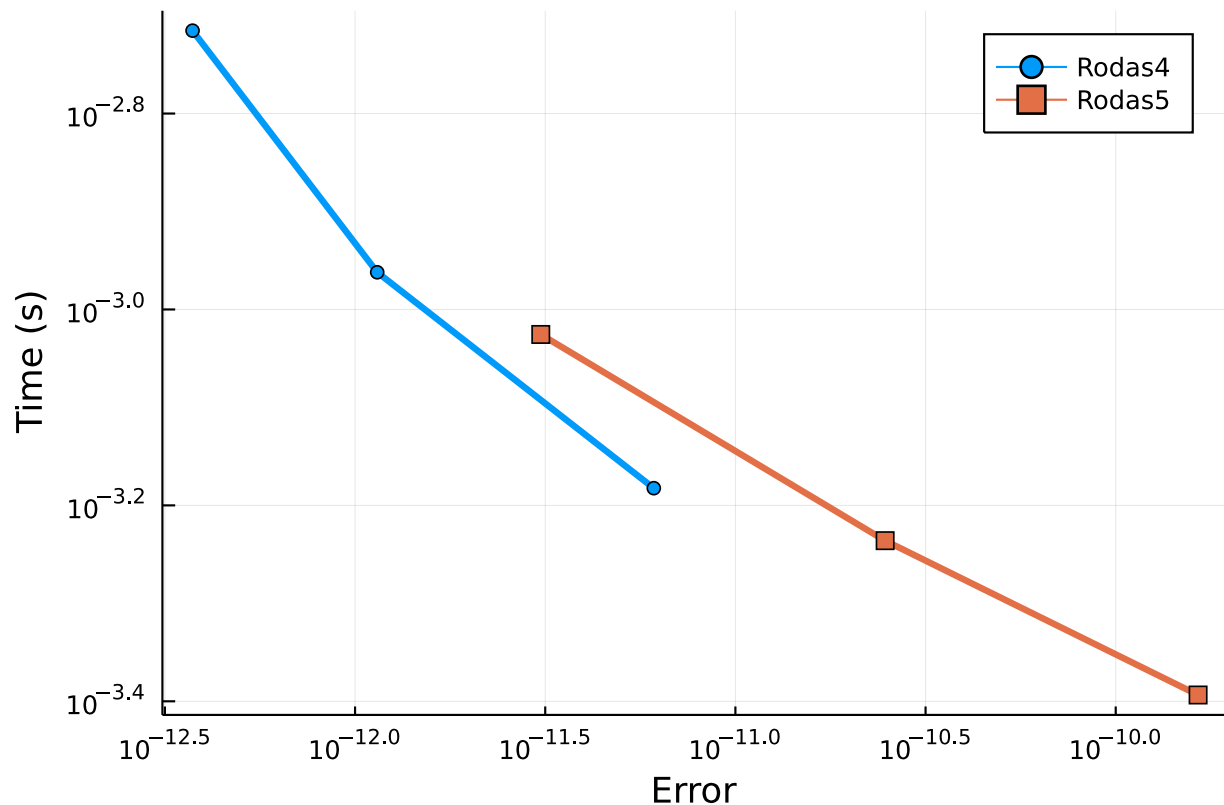


```

abstols = 1.0 ./ 10.0 .^ (10:12)
reltols = 1.0 ./ 10.0 .^ (7:9)

setups = [Dict(:alg=>Rodas4())
          Dict(:alg=>Rodas5())]
names = ["Rodas4" "Rodas5"]
wp = WorkPrecisionSet(prob,abstols,reltols,setups;names=names,
                      save_everystep=false,appxsol=test_sol,maxiters=Int(1e5),numruns=10)
plot(wp)

```



0.2.3 Conclusion

At high tolerances, **Rosenbrock23** and **lsoda** hit the the error estimates and are fast. At lower tolerances and normal user tolerances, **Rodas4** and **Rodas5** are extremely fast. **lsoda** does quite well across both ends. When you get down to `reltol=1e-9` radau begins to become as efficient as **Rodas4**, and it continues to do well below that.

0.3 Appendix

These benchmarks are a part of the SciMLBenchmarks.jl repository, found at: <https://github.com/SciML/SciMLBenchmarks.jl>. For more information on high-performance scientific machine learning, check out the SciML Open Source Software Organization <https://sciml.ai>.

To locally run this benchmark, do the following commands:

```
using SciMLBenchmarks
SciMLBenchmarks.weave_file("benchmarks/StiffODE", "ROBER.jmd")
```

Computer Information:

```
Julia Version 1.6.1
Commit 6aaedecc44 (2021-04-23 05:59 UTC)
Platform Info:
  OS: Linux (x86_64-pc-linux-gnu)
  CPU: Intel(R) Core(TM) i7-9700K CPU @ 3.60GHz
```

```

WORD_SIZE: 64
LIBM: libopenlibm
LLVM: libLLVM-11.0.1 (ORCJIT, skylake)
Environment:
JULIA_DEPOT_PATH = /root/.cache/julia-buildkite-plugin/depots/5b300254-1738-4989-ae0
JULIA_NUM_THREADS = 3

```

Package Information:

```

      Status `~/var/lib/buildkite-agent/builds/rtx2070-gpuci1-julia-csail-mit-edu/julia
[f3b72e0c] DiffEqDevTools v2.27.2
[5a33fad7] GeometricIntegratorsDiffEq v0.2.0
[7f56f5a3] LSODA v0.7.0
[c030b06c] ODE v2.13.0
[09606e27] ODEInterfaceDiffEq v3.10.0
[1dea7af3] OrdinaryDiffEq v5.53.1
[65888b18] ParameterizedFunctions v5.10.0
[91a5bcd] Plots v1.13.2
[31c91b34] SciMLBenchmarks v0.1.0 `../..#`
[c3572dad] Sundials v4.4.3
[a759f4b9] TimerOutputs v0.5.8
[37e2e46d] LinearAlgebra

```

And the full manifest:

```

      Status `~/var/lib/buildkite-agent/builds/rtx2070-gpuci1-julia-csail-mit-edu/julia
[c3fe647b] AbstractAlgebra v0.16.0
[621f4979] AbstractFFTs v1.0.1
[1520ce14] AbstractTrees v0.3.4
[79e6a3ab] Adapt v3.3.0
[4c88cf16] Aqua v0.5.0
[ec485272] ArnoldiMethod v0.1.0
[4fba245c] ArrayInterface v3.1.11
[4c555306] ArrayLayouts v0.4.12
[9e28174c] BinDeps v1.0.2
[b99e7846] BinaryProvider v0.5.10
[a74b3585] Blosc v0.7.0
[fa961155] CEnum v0.4.1
[d360d2e6] ChainRulesCore v0.9.41
[b630d9fa] CheapThreads v0.2.3
[35d6a980] ColorSchemes v3.12.1
[3da002f7] ColorTypes v0.11.0
[5ae59095] Colors v0.12.8
[861a8166] Combinatorics v1.0.2
[38540f10] CommonSolve v0.2.0
[bbf7d656] CommonSubexpressions v0.3.0
[34da2185] Compat v3.28.0

```

[8f4d0f93] Conda v1.5.2
[187b0558] ConstructionBase v1.2.1
[d38c429a] Contour v0.5.7
[717857b8] DSP v0.6.10
[9a962f9c] DataAPI v1.6.0
[864edb3b] DataStructures v0.18.9
[e2d170a0] DataValueInterfaces v1.0.0
[55939f99] DecFP v1.1.0
[2b5f629d] DiffEqBase v6.61.0
[f3b72e0c] DiffEqDevTools v2.27.2
[c894b116] DiffEqJump v6.14.1
[77a26b50] DiffEqNoiseProcess v5.7.2
[163ba53b] DiffResults v1.0.3
[b552c78f] DiffRules v1.0.2
[b4f34e82] Distances v0.10.3
[31c24e10] Distributions v0.24.18
[ffbed154] DocStringExtensions v0.8.4
[e30172f5] Documenter v0.26.3
[d4d017d3] ExponentialUtilities v1.8.4
[e2ba6199] ExprTools v0.1.3
[8f5d6c58] EzXML v1.1.0
[c87230d0] FFMPEG v0.4.0
[7a1cc6ca] FFTW v1.4.1
[7034ab61] FastBroadcast v0.1.5
[9aa1b823] FastClosures v0.3.2
[442a2c76] FastGaussQuadrature v0.4.7
[057dd010] FastTransforms v0.11.3
[1a297f60] FillArrays v0.10.2
[6a86dc24] FiniteDiff v2.8.0
[53c48c17] FixedPointNumbers v0.8.4
[59287772] Formatting v0.4.2
[f6369f11] ForwardDiff v0.10.18
[069b7b12] FunctionWrappers v1.1.2
[28b8d3ca] GR v0.57.4
[14197337] GenericLinearAlgebra v0.2.5
[dcce2d33] GeometricIntegrators v0.6.2
[5a33fad7] GeometricIntegratorsDiffEq v0.2.0
[5c1252a2] GeometryBasics v0.3.12
[d7ba0133] Git v1.2.1
[42e2da0e] Grisu v1.0.2
[f67ccb44] HDF5 v0.14.3
[cd3eb016] HTTP v0.9.8
[eafb193a] Highlights v0.4.5
[0e44f5e4] Hwloc v2.0.0
[7073ff75] IJulia v1.23.2
[b5f81e59] IOCapture v0.1.1
[615f187c] IfElse v0.1.0
[d25df0c9] Inflate v0.1.2
[83e8ac13] IniFile v0.5.0

[d8418881] Intervals v1.5.0
[c8e1da08] IterTools v1.3.0
[42fd0dbc] IterativeSolvers v0.9.0
[82899510] IteratorInterfaceExtensions v1.0.0
[692b3bcd] JLLWrappers v1.3.0
[682c06a0] JSON v0.21.1
[7f56f5a3] LSODA v0.7.0
[b964fa9f] LaTeXStrings v1.2.1
[2ee39098] LabelledArrays v1.6.0
[23fbe1c1] Latexify v0.15.5
[093fc24a] LightGraphs v1.3.5
[d3d80556] LineSearches v7.1.1
[2ab3a3ac] LogExpFunctions v0.2.3
[bdcacae8] LoopVectorization v0.12.18
[1914dd2f] MacroTools v0.5.6
[739be429] MbedTLS v1.0.3
[442fdcdd] Measures v0.3.1
[c03570c3] Memoize v0.4.4
[e1d29d7a] Missings v1.0.0
[78c3b35d] Mocking v0.7.1
[961ee093] ModelingToolkit v5.16.0
[46d2c3a1] MuladdMacro v0.2.2
[ffc61752] Mustache v1.0.10
[d41bc354] NLSolversBase v7.8.0
[2774e3e8] NLSolve v4.5.1
[77ba4419] NaNMath v0.3.5
[8913a72c] NonlinearSolve v0.3.8
[c030b06c] ODE v2.13.0
[54ca160b] ODEInterface v0.5.0
[09606e27] ODEInterfaceDiffEq v3.10.0
[6fe1bfb0] OffsetArrays v1.8.0
[429524aa] Optim v1.3.0
[bac558e1] OrderedCollections v1.4.0
[1dea7af3] OrdinaryDiffEq v5.53.1
[90014a1f] PDMats v0.11.0
[65888b18] ParameterizedFunctions v5.10.0
[d96e819e] Parameters v0.12.2
[69de0a69] Parsers v1.1.0
[ccf2f8ad] PlotThemes v2.0.1
[995b91a9] PlotUtils v1.0.10
[91a5bcdd] Plots v1.13.2
[e409e4f3] PoissonRandom v0.4.0
[f27b6e38] Polynomials v1.2.1
[85a6dd25] PositiveFactorizations v0.2.4
[21216c6a] Preferences v1.2.2
[92933f4c] ProgressMeter v1.6.2
[1fd47b50] QuadGK v2.4.1
[74087812] Random123 v1.3.1
[fb686558] RandomExtensions v0.4.3

[e6cf234a] RandomNumbers v1.4.0
[3cdcf5f2] RecipesBase v1.1.1
[01d81517] RecipesPipeline v0.3.2
[731186ca] RecursiveArrayTools v2.11.3
[f2c3362d] RecursiveFactorization v0.1.12
[189a3867] Reexport v0.2.0
[ae029012] Requires v1.1.3
[ae5879a3] ResettableStacks v1.1.0
[79098fc4] Rmath v0.7.0
[47965b36] RootedTrees v1.0.0
[7e49a35a] RuntimeGeneratedFunctions v0.5.2
[476501e8] SLEEF Pirates v0.6.17
[1bc83da4] SafeTestsets v0.0.1
[0bca4576] SciMLBase v1.13.2
[31c91b34] SciMLBenchmarks v0.1.0 `.../...#`
[6c6a2e73] Scratch v1.0.3
[efcf1570] Setfield v0.7.0
[992d4aef] Showoff v1.0.3
[699a6c99] SimpleTraits v0.9.3
[b85f4697] SoftGlobalScope v1.1.0
[a2af1166] SortingAlgorithms v1.0.0
[47a9eef4] SparseDiffTools v1.13.2
[276daf66] SpecialFunctions v0.10.3
[a25cea48] SpecialPolynomials v0.1.0
[aedffcd0] Static v0.2.4
[90137ffa] StaticArrays v1.1.3
[82ae8749] StatsAPI v1.0.0
[2913bbd2] StatsBase v0.33.8
[4c63d2b9] StatsFuns v0.9.8
[7792a7ef] StrideArraysCore v0.1.7
[09ab397b] StructArrays v0.5.1
[c3572dad] Sundials v4.4.3
[d1185830] SymbolicUtils v0.11.2
[0c5d862f] Symbolics v0.1.25
[3783bdb8] TableTraits v1.0.1
[bd369af6] Tables v1.4.2
[8290d209] ThreadingUtilities v0.4.1
[f269a46b] TimeZones v1.5.4
[a759f4b9] TimerOutputs v0.5.8
[c751599d] ToeplitzMatrices v0.6.3
[a2a6695c] TreeViews v0.3.0
[30578b45] URIParser v0.4.1
[5c2747f8] URIs v1.3.0
[3a884ed6] UnPack v1.0.2
[1986cc42] Unitful v1.7.0
[3d5dd08c] VectorizationBase v0.19.37
[81def892] VersionParsing v1.2.0
[19fa3120] VertexSafeGraphs v0.1.2
[44d3d7a6] Weave v0.10.8

[ddb6d928] YAML v0.4.6
 [c2297ded] ZMQ v1.2.1
 [700de1a5] ZygoteRules v0.2.1
 [0b7ba130] Blosc_jll v1.14.3+1
 [6e34b625] Bzip2_jll v1.0.6+5
 [83423d85] Cairo_jll v1.16.0+6
 [47200ebd] DecFP_jll v2.0.2+0
 [5ae413db] EarCut_jll v2.1.5+1
 [2e619515] Expat_jll v2.2.7+6
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 [f5851436] FFTW_jll v3.3.9+7
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 [a3f928ae] Fontconfig_jll v2.13.1+14
 [d7e528f0] FreeType2_jll v2.10.1+5
 [559328eb] FriBidi_jll v1.0.5+6
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 [f8c6e375] Git_jll v2.31.0+0
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 [aacddb02] JpegTurbo_jll v2.0.1+3
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 [d4300ac3] Libgcrypt_jll v1.8.5+4
 [7e76a0d4] Libglvnd_jll v1.3.0+3
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 [38a345b3] Libuuid_jll v2.34.0+7
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