VanDerPol Work-Precision Diagrams

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```
using OrdinaryDiffEq, DiffEqDevTools, Sundials, ParameterizedFunctions, Plots, ODE,
ODEInterfaceDiffEq, LSODA
gr()
using LinearAlgebra
LinearAlgebra.BLAS.set_num_threads(1)

van = @ode_def begin
  dy = μ*((1-x^2)*y - x)
  dx = 1*y
end μ

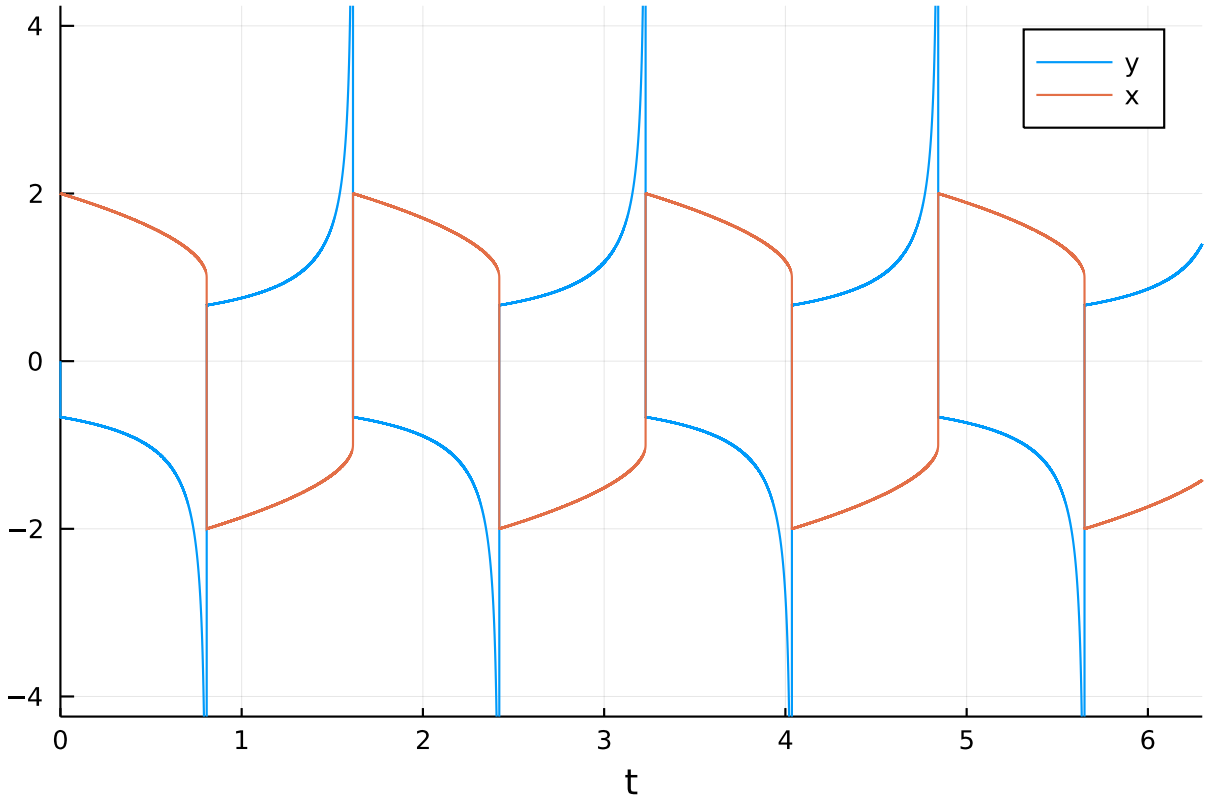
prob = ODEProblem(van,[0;2.],(0.0,6.3),1e6)
abstols = 1.0 ./ 10.0 .^ (5:9)
reltols = 1.0 ./ 10.0 .^ (2:6)

sol = solve(prob,CVODE_BDF(),abstol=1/10^14,reltol=1/10^14)
test_sol = TestSolution(sol)

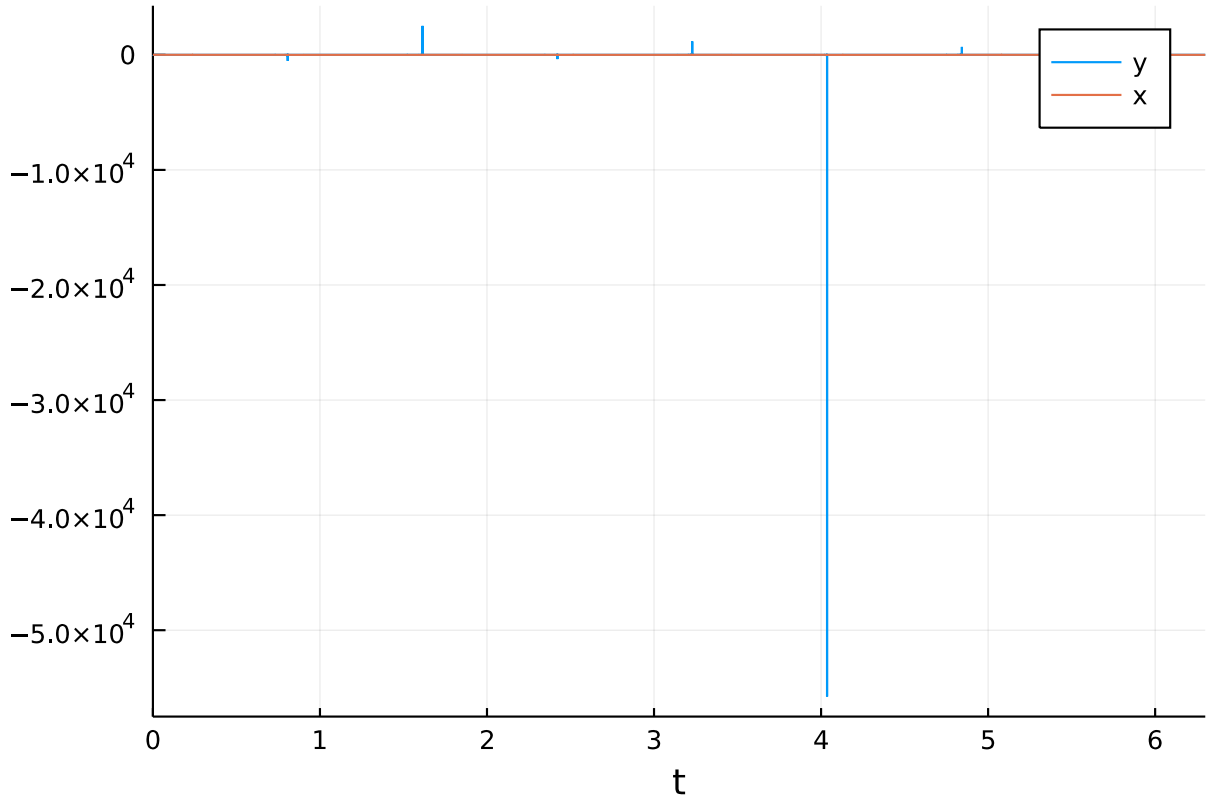
retcode: Success
Interpolation: 3rd order Hermite
t: nothing
u: nothing
```

0.0.1 Plot Test

```
plot(sol,ylim=[-4;4])
```




```
plot(sol)
```



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=1/1000)
#catch e
#    println(e)
#end
```

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

```
sol = solve(prob,ARKODE(),abstol=1e-4,reltol=1e-2);

sol = solve(prob,ARKODE(nonlinear_convergence_coefficient =
1e-6),abstol=1e-4,reltol=1e-1);

sol = solve(prob,ARKODE(order=3),abstol=1e-4,reltol=1e-1);

sol = solve(prob,ARKODE(nonlinear_convergence_coefficient =
1e-6,order=3),abstol=1e-4,reltol=1e-1);

sol = solve(prob,ARKODE(order=5,nonlinear_convergence_coefficient =
1e-3),abstol=1e-4,reltol=1e-1);

sol = solve(prob,ARKODE(order=5,nonlinear_convergence_coefficient =
1e-4),abstol=1e-4,reltol=1e-1);
```

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

```
setups = [
          #Dict(:alg=>ROCK2())    #Unstable
          #Dict(:alg=>ROCK4())    #needs more iterations
          #Dict(:alg=>ESERK5()),
          ]
```

```
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)
```

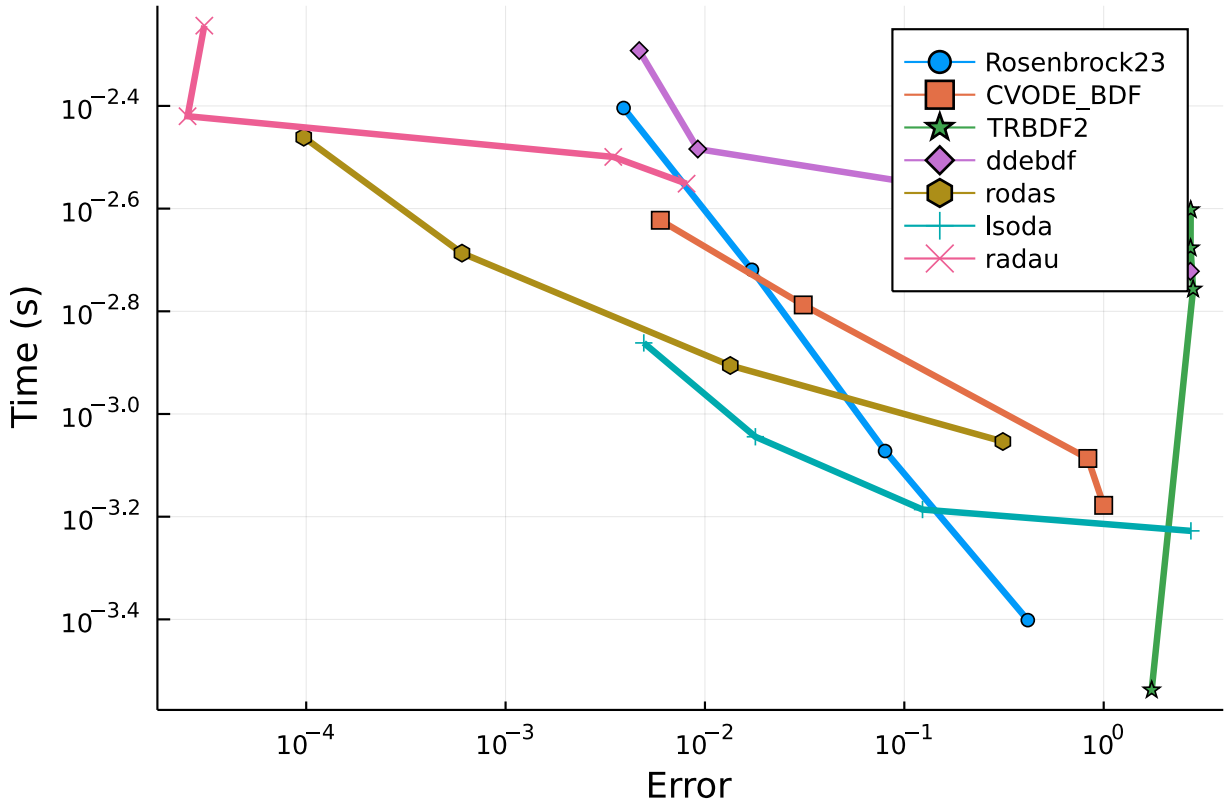
0.2 Low Order and High Tolerance

This tests the case where accuracy is not needed as much and quick robust solutions are necessary. Note that `ARKODE`'s convergence coefficient must be lowered to `1e-7` in order to converge.

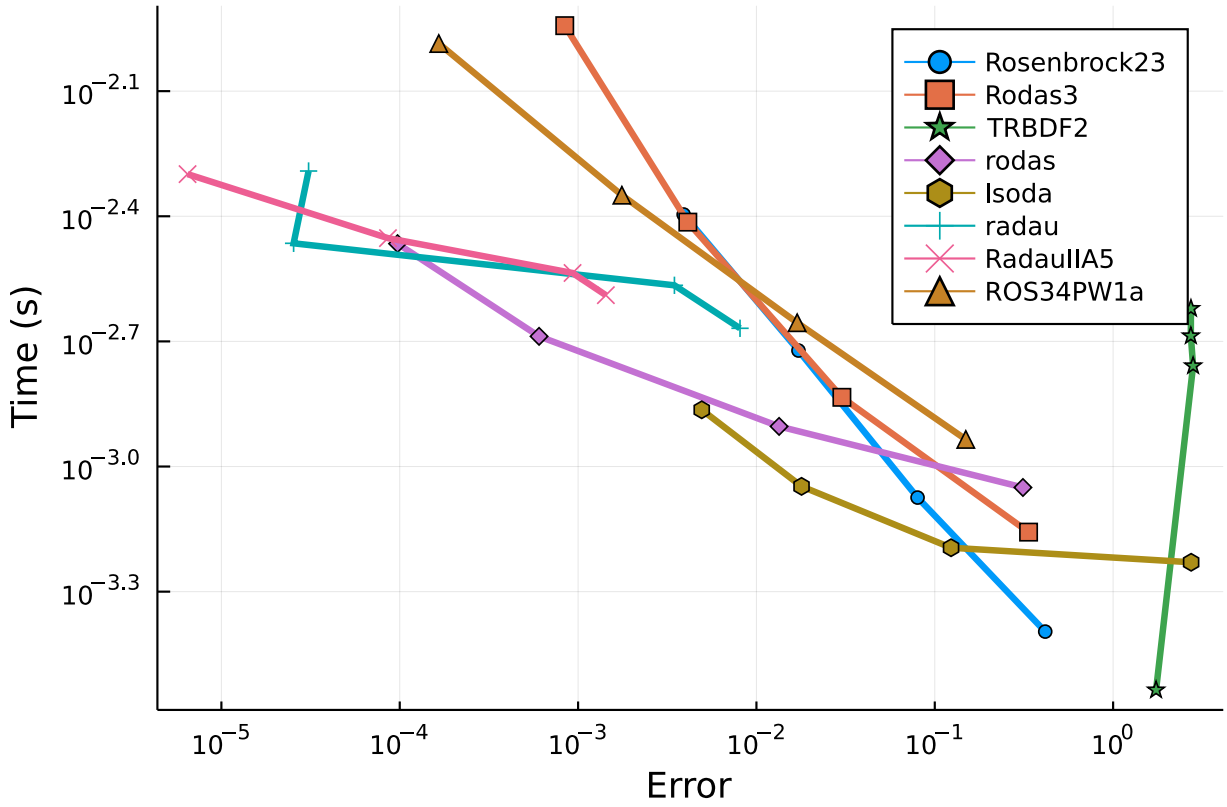
Final timepoint error This measures the efficiency to get the value at the endpoint correct.

```
abstols = 1.0 ./ 10.0 .^ (4:7)
reltols = 1.0 ./ 10.0 .^ (1:4)

setups = [Dict(:alg=>Rosenbrock23()),
          Dict(:alg=>CVODE_BDF()),
          Dict(:alg=>TRBDF2()),
          Dict(:alg=>ddebdf()),
          Dict(:alg=>rodas()),
          Dict(:alg=>lsoda()),
          Dict(:alg=>radau())]
wp = WorkPrecisionSet(prob,abstols,reltols,setups;
                      save_everystep=false,appxsol=test_sol,maxiters=Int(1e5),seconds=5)
plot(wp)
```

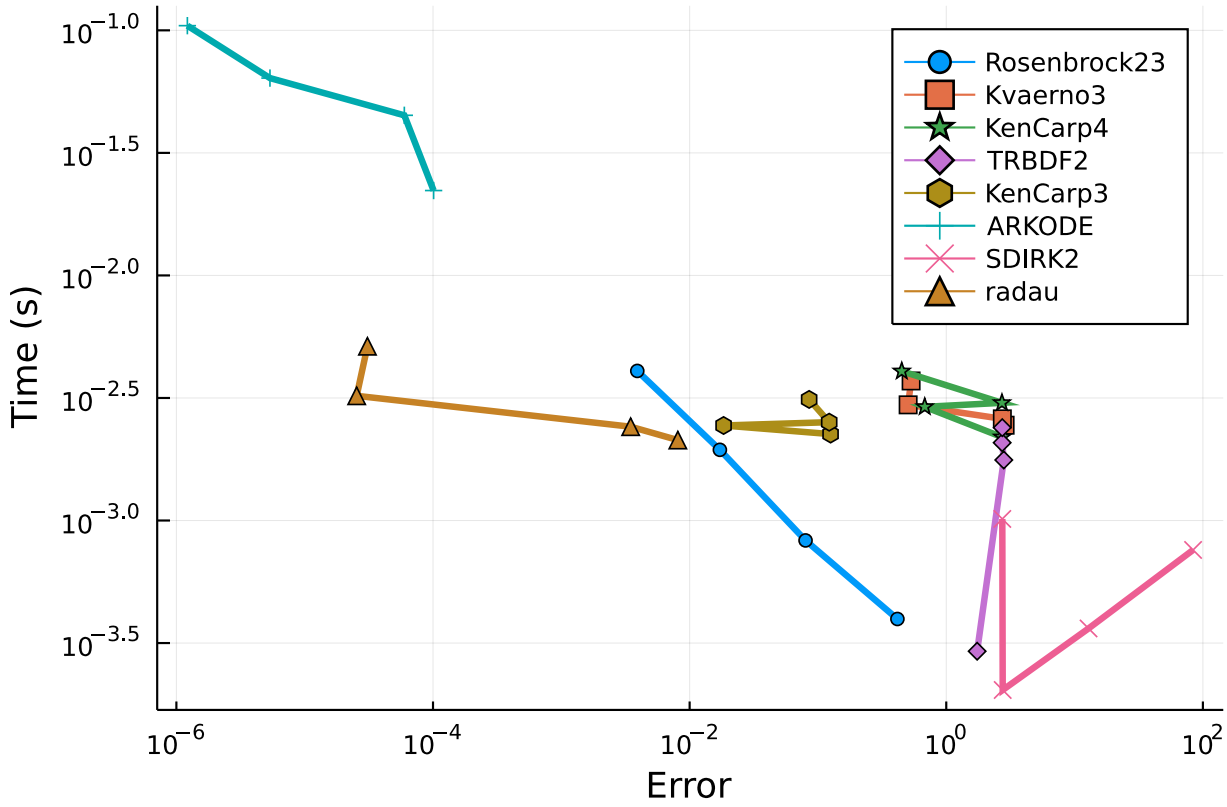



```
setups = [Dict(:alg=>Rosenbrock23()),
          Dict(:alg=>Rodas3()),
          Dict(:alg=>TRBDF2()),
          Dict(:alg=>rodas()),
          Dict(:alg=>lsoda()),
          Dict(:alg=>radau()),
          Dict(:alg=>RadauIIA5()),
          Dict(:alg=>ROS34PW1a()),
          ]
gr()
wp = WorkPrecisionSet(prob,abstols,reltols,setups;
                      save_everystep=false,appxsol=test_sol,maxiters=Int(1e5),numruns=10)
plot(wp)
```



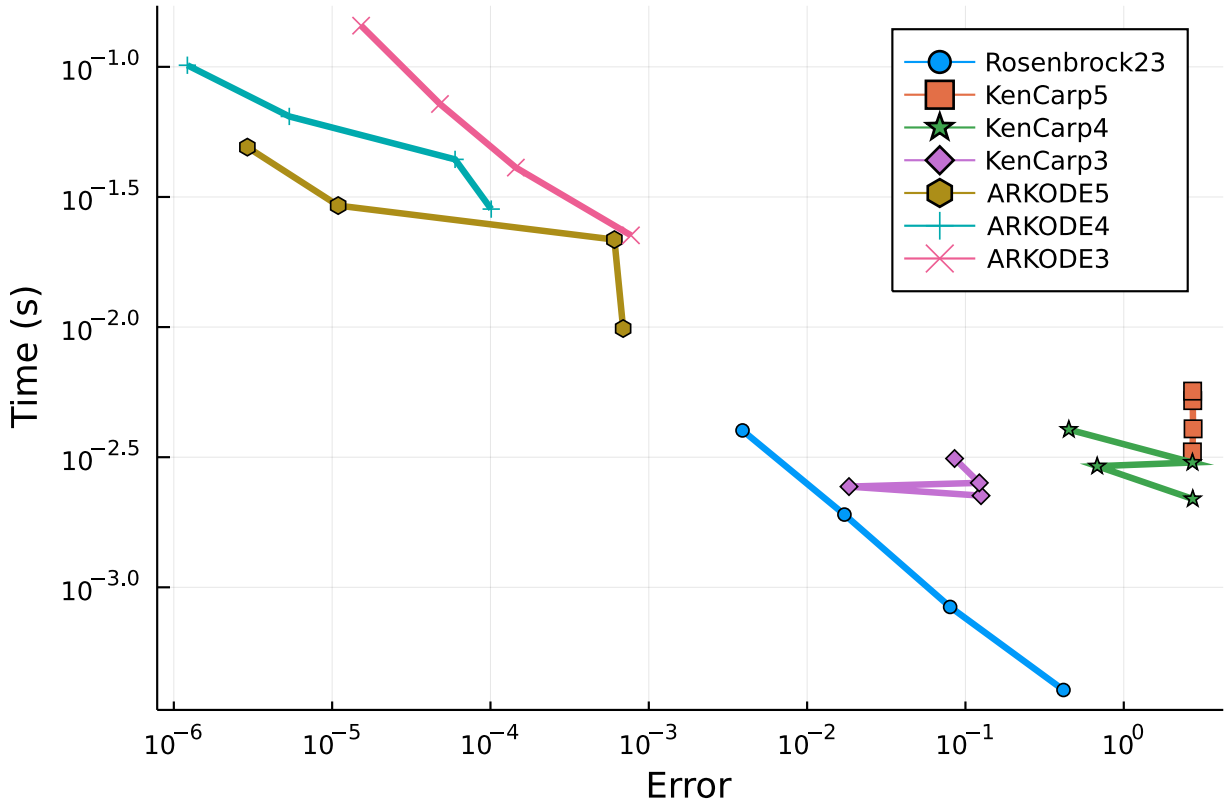

```
setups = [Dict(:alg=>Rosenbrock23()),
          Dict(:alg=>Kvaerno3()),
          Dict(:alg=>KenCarp4()),
          Dict(:alg=>TRBDF2()),
          Dict(:alg=>KenCarp3()),
          Dict(:alg=>ARKODE(nonlinear_convergence_coefficient = 1e-6)),
          Dict(:alg=>SDIRK2()),
          Dict(:alg=>radau())]
names = ["Rosenbrock23" "Kvaerno3" "KenCarp4" "TRBDF2" "KenCarp3" "ARKODE" "SDIRK2"
"radau"]
wp = WorkPrecisionSet(prob,abstols,reltols,setups;

names=names,save_everystep=false,appxsol=test_sol,maxiters=Int(1e5),seconds=5)
plot(wp)
```

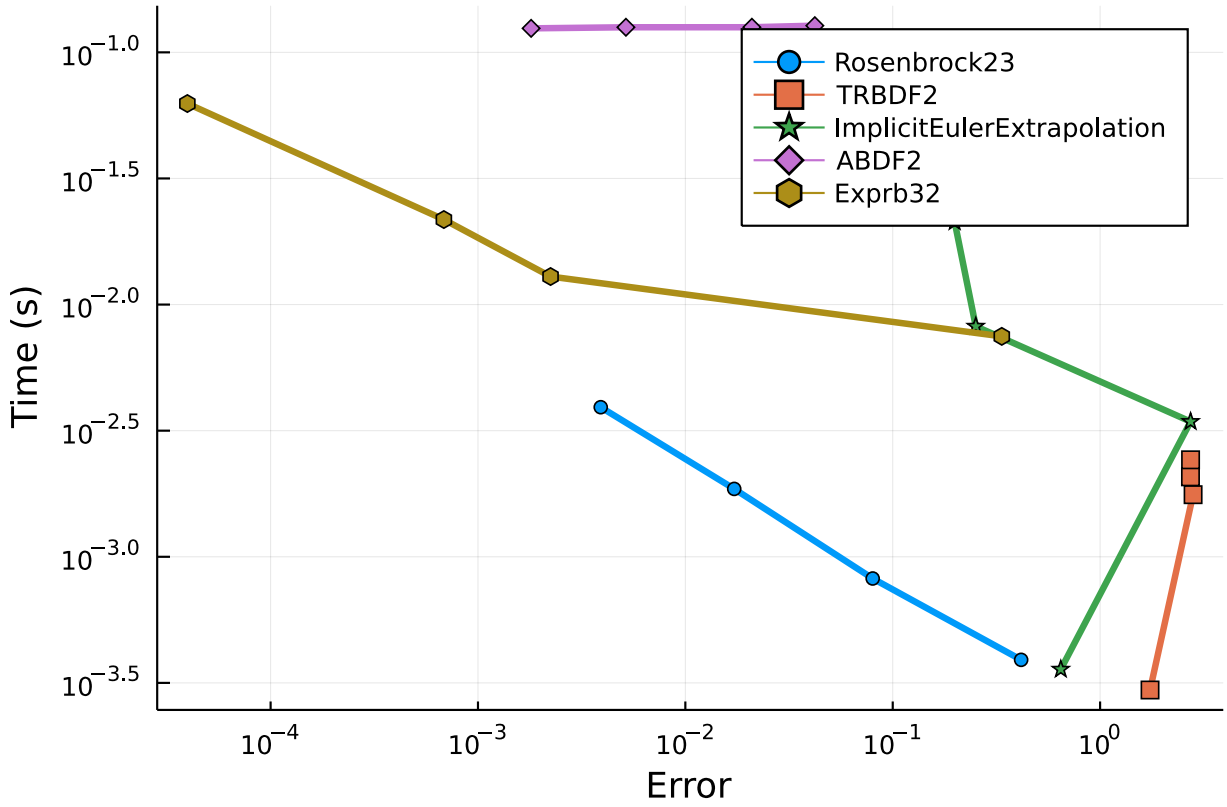



```
setups = [Dict(:alg=>Rosenbrock23()),
          Dict(:alg=>KenCarp5()),
          Dict(:alg=>KenCarp4()),
          Dict(:alg=>KenCarp3()),
          Dict(:alg=>ARKODE(order=5,nonlinear_convergence_coefficient = 1e-4)),
          Dict(:alg=>ARKODE(nonlinear_convergence_coefficient = 1e-6)),
          Dict(:alg=>ARKODE(nonlinear_convergence_coefficient = 1e-6,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),seconds=5)
plot(wp)
```




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

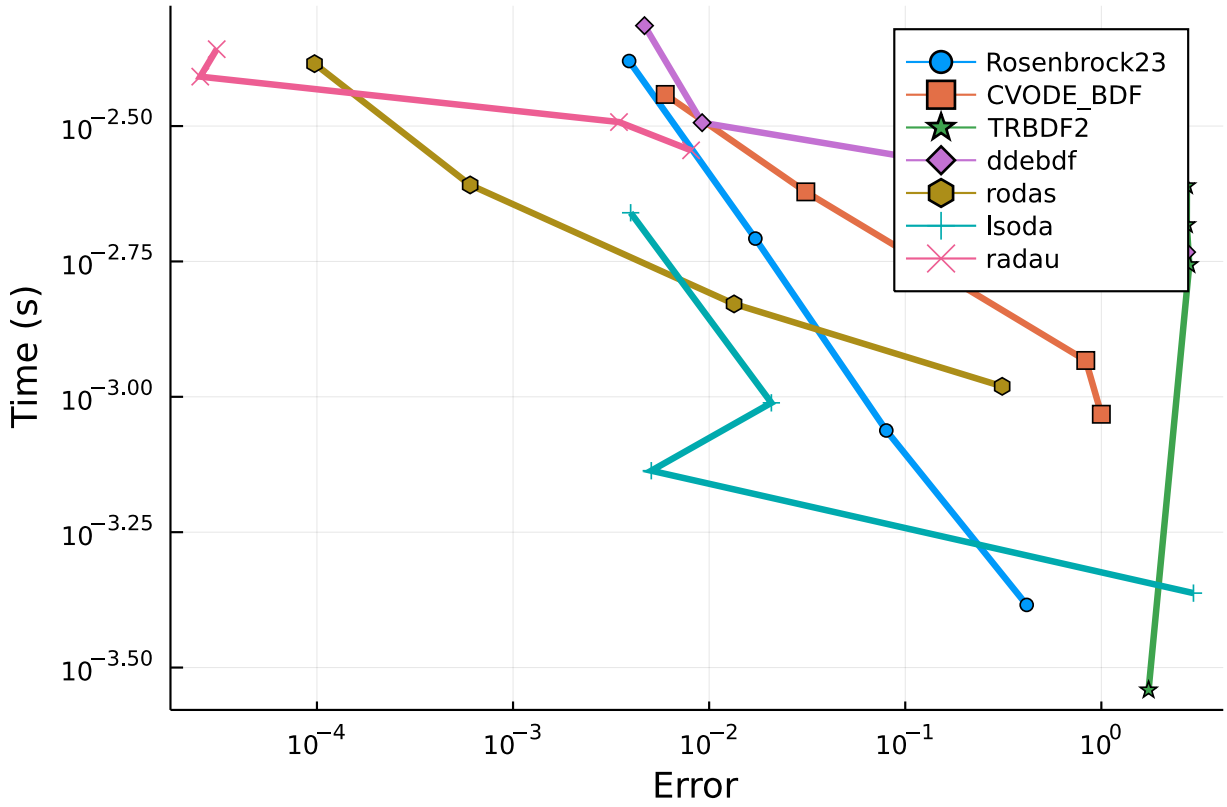


Notice that `KenCarp4` is the same overarching algorithm as `ARKODE` here (with major differences to stage predictors and adaptivity though). In this case, `KenCarp4` is more robust and more efficient than `ARKODE`. `CVODE_BDF` does quite well here, which is unusual for it on small equations. You can see that the low-order Rosenbrock methods `Rosenbrock23` and `Rodas3` dominate this test.

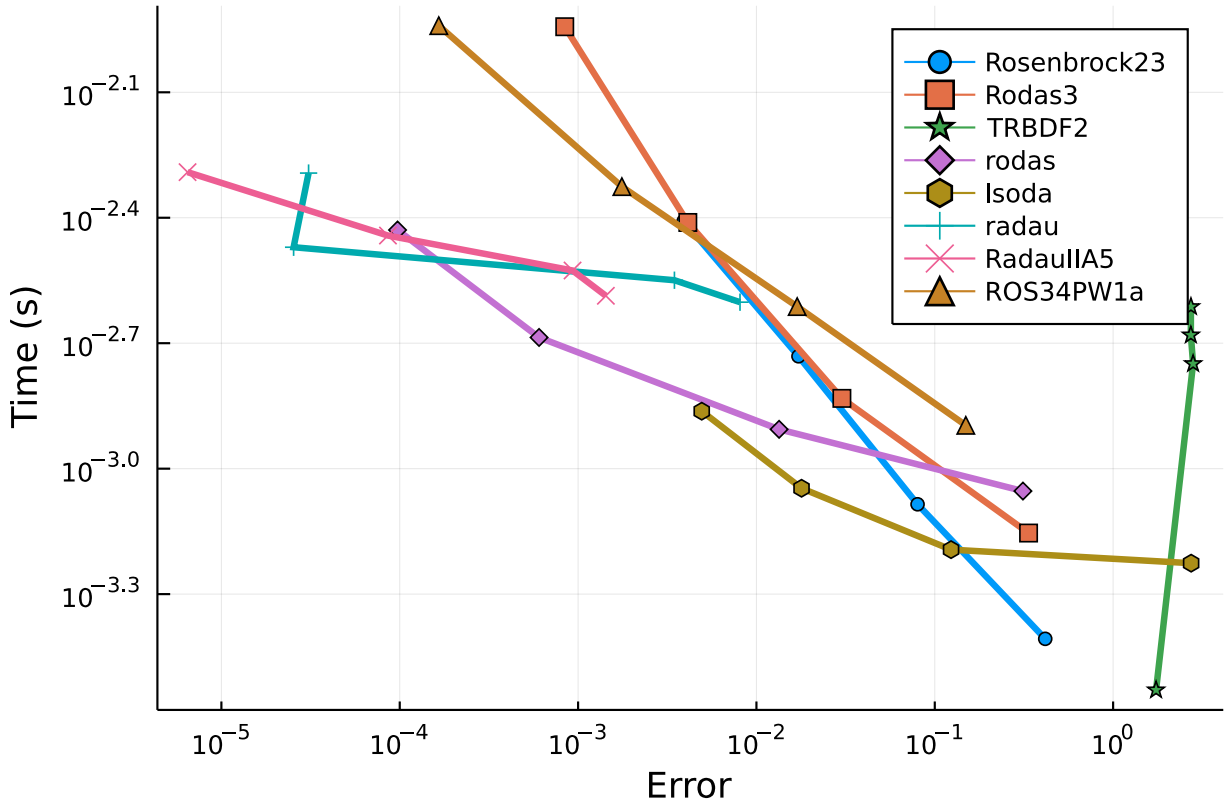
Timeseries error Now we measure the average error of the timeseries.

```
abstols = 1.0 ./ 10.0 .^ (4:7)
reltols = 1.0 ./ 10.0 .^ (1:4)

setups = [Dict(:alg=>Rosenbrock23()),
          Dict(:alg=>CVODE_BDF()),
          Dict(:alg=>TRBDF2()),
          Dict(:alg=>ddebdf()),
          Dict(:alg=>rodas()),
          Dict(:alg=>lsoda()),
          Dict(:alg=>radau())]
wp = WorkPrecisionSet(prob,abstols,reltols,setups;
                      error_estimator=:l2,appxsol=test_sol,maxiters=Int(1e5),seconds=5)
plot(wp)
```

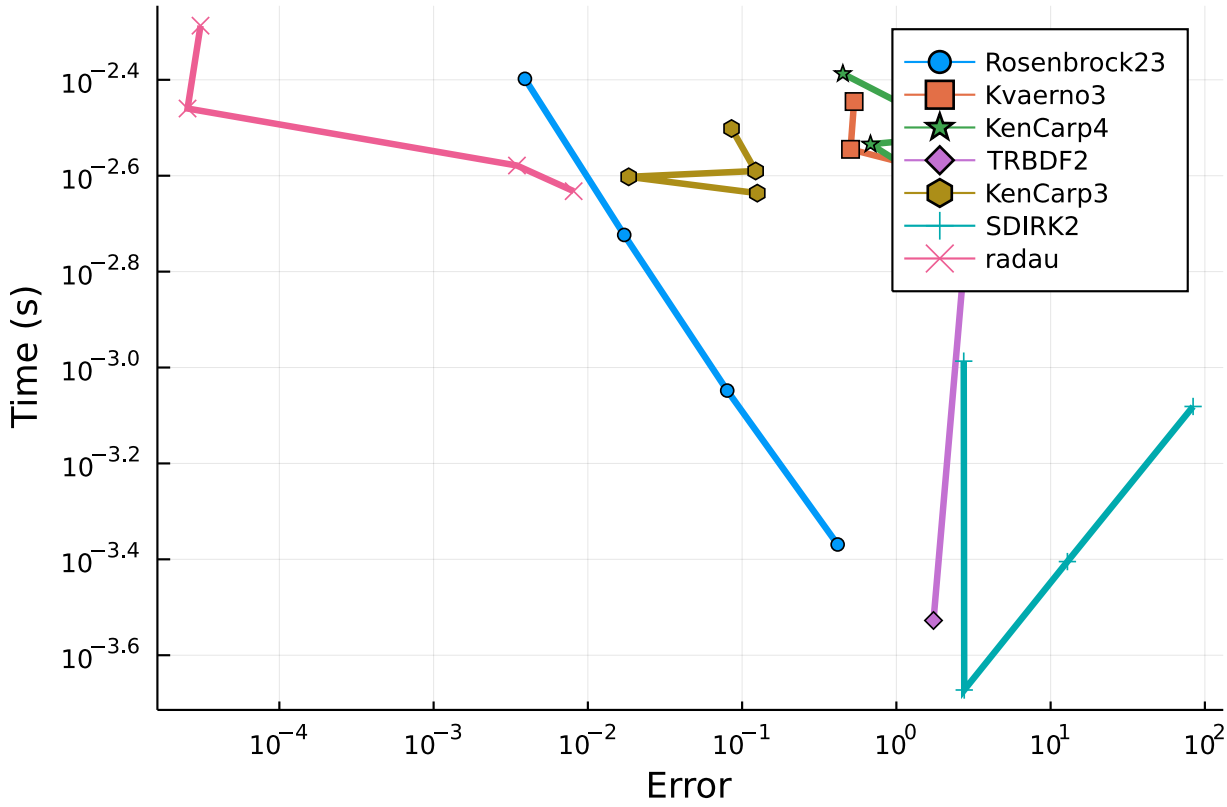



```
setups = [Dict(:alg=>Rosenbrock23()),
          Dict(:alg=>Rodas3()),
          Dict(:alg=>TRBDF2()),
          Dict(:alg=>rodas()),
          Dict(:alg=>lsoda()),
          Dict(:alg=>radau()),
          Dict(:alg=>RadauIIA5()),
          Dict(:alg=>ROS34PW1a()),
          ]
gr()
wp = WorkPrecisionSet(prob,abstols,reltols,setups;error_estimator=:l2,
                      save_everystep=false,appxsol=test_sol,maxiters=Int(1e5),numruns=10)
plot(wp)
```

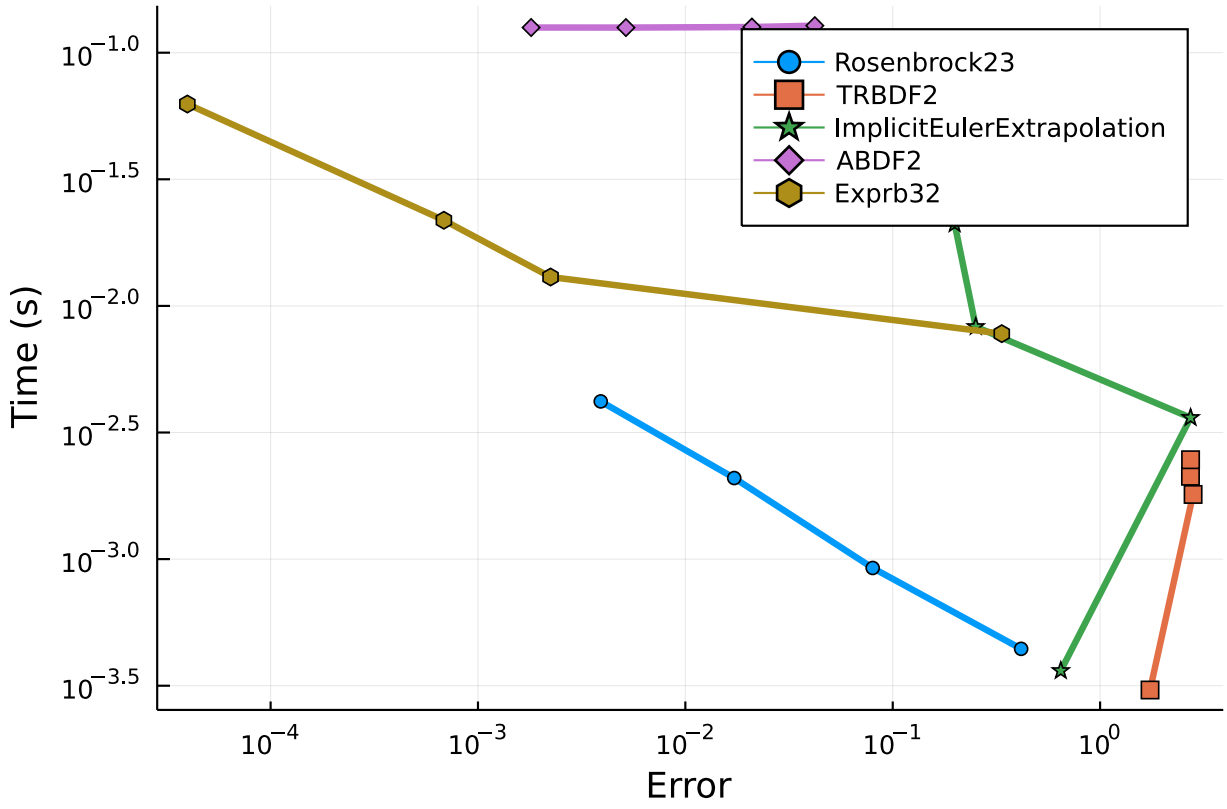



```
setups = [Dict(:alg=>Rosenbrock23(),:dense=>false),
          Dict(:alg=>Kvaerno3(),:dense=>false),
          Dict(:alg=>KenCarp4(),:dense=>false),
          Dict(:alg=>TRBDF2(),:dense=>false),
          Dict(:alg=>KenCarp3(),:dense=>false),
          Dict(:alg=>SDIRK2(),:dense=>false),
          Dict(:alg=>radau())]
names = ["Rosenbrock23" "Kvaerno3" "KenCarp4" "TRBDF2" "KenCarp3" "SDIRK2" "radau"]
wp = WorkPrecisionSet(prob,abstols,reltols,setups;

names=names,appxsol=test_sol,maxiters=Int(1e5),error_estimator=:l2,seconds=5)
plot(wp)
```



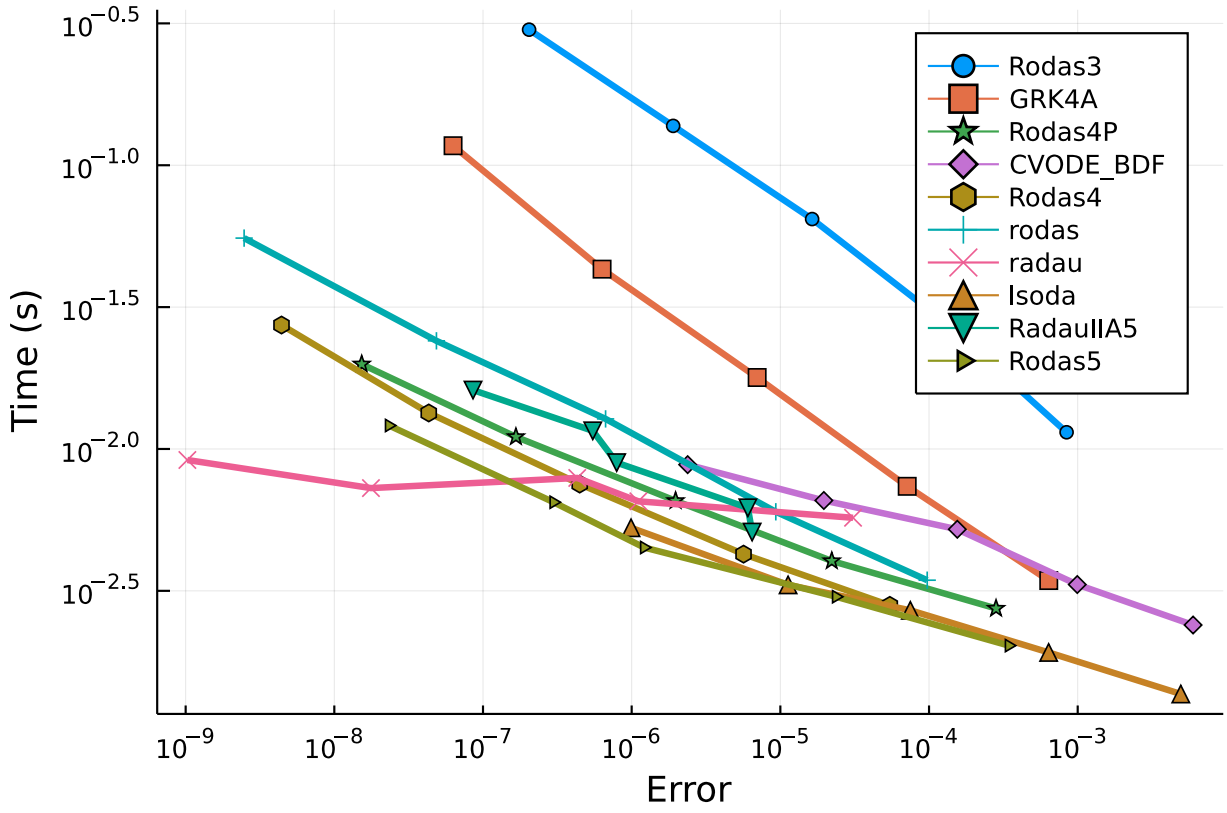

```
setups = [Dict(:alg=>Rosenbrock23()),
          Dict(:alg=>TRBDF2()),
          Dict(:alg=>ImplicitEulerExtrapolation()),
          #Dict(:alg=>ImplicitDeuflhardExtrapolation()), # Diverges
          #Dict(:alg=>ImplicitHairerWannerExtrapolation()), # Diverges
          Dict(:alg=>ABDF2()),
    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



0.2.1 Higher accuracy tests

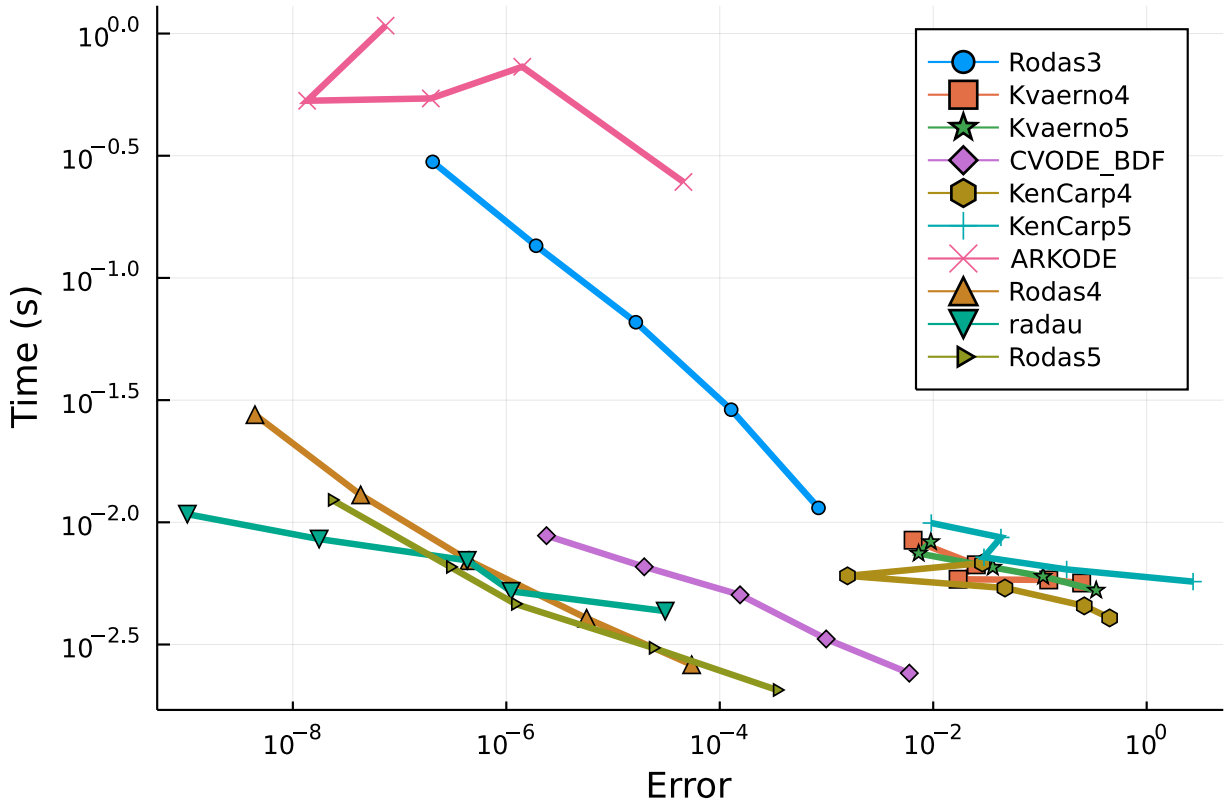
Now we transition to higher accracy tests. In this domain higher order methods are stable and much more efficient.

```
abstols = 1.0 ./ 10.0 .^ (7:11)
reltols = 1.0 ./ 10.0 .^ (4:8)
setups = [Dict(:alg=>Rodas3()),
          Dict(:alg=>GRK4A()),
          Dict(:alg=>Rodas4P()),
          Dict(:alg=>CVODE_BDF()),
          Dict(:alg=>Rodas4()),
          Dict(:alg=>rodas()),
          Dict(:alg=>radau()),
          Dict(:alg=>lsoda()),
          Dict(:alg=>RadauIIA5()),
          Dict(:alg=>Rodas5())]
wp = WorkPrecisionSet(prob,abstols,reltols,setups;
                      save_everystep=false,appxsol=test_sol,maxiters=Int(1e6),seconds=5)
plot(wp)
```

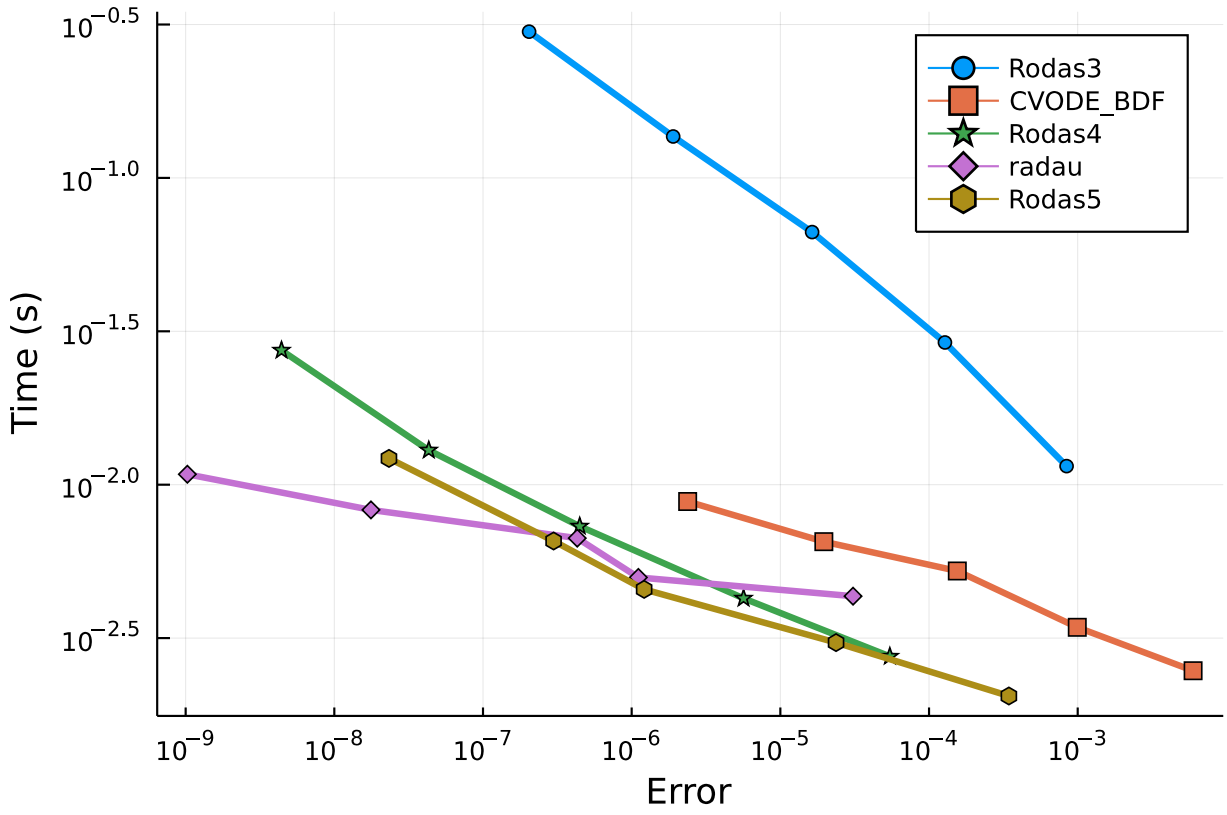



```
abstols = 1.0 ./ 10.0 .^ (7:11)
reltols = 1.0 ./ 10.0 .^ (4:8)
setups = [Dict(:alg=>Rodas3()),
          Dict(:alg=>Kvaerno4()),
          Dict(:alg=>Kvaerno5()),
          Dict(:alg=>CVODE_BDF()),
          Dict(:alg=>KenCarp4()),
          Dict(:alg=>KenCarp5()),
          Dict(:alg=>ARKODE()),
          Dict(:alg=>Rodas4()),
          Dict(:alg=>radau()),
          Dict(:alg=>Rodas5())]
names = ["Rodas3" "Kvaerno4" "Kvaerno5" "CVODE_BDF" "KenCarp4" "KenCarp5" "ARKODE"
"Rodas4" "radau" "Rodas5"]
wp = WorkPrecisionSet(prob,abstols,reltols,setups;

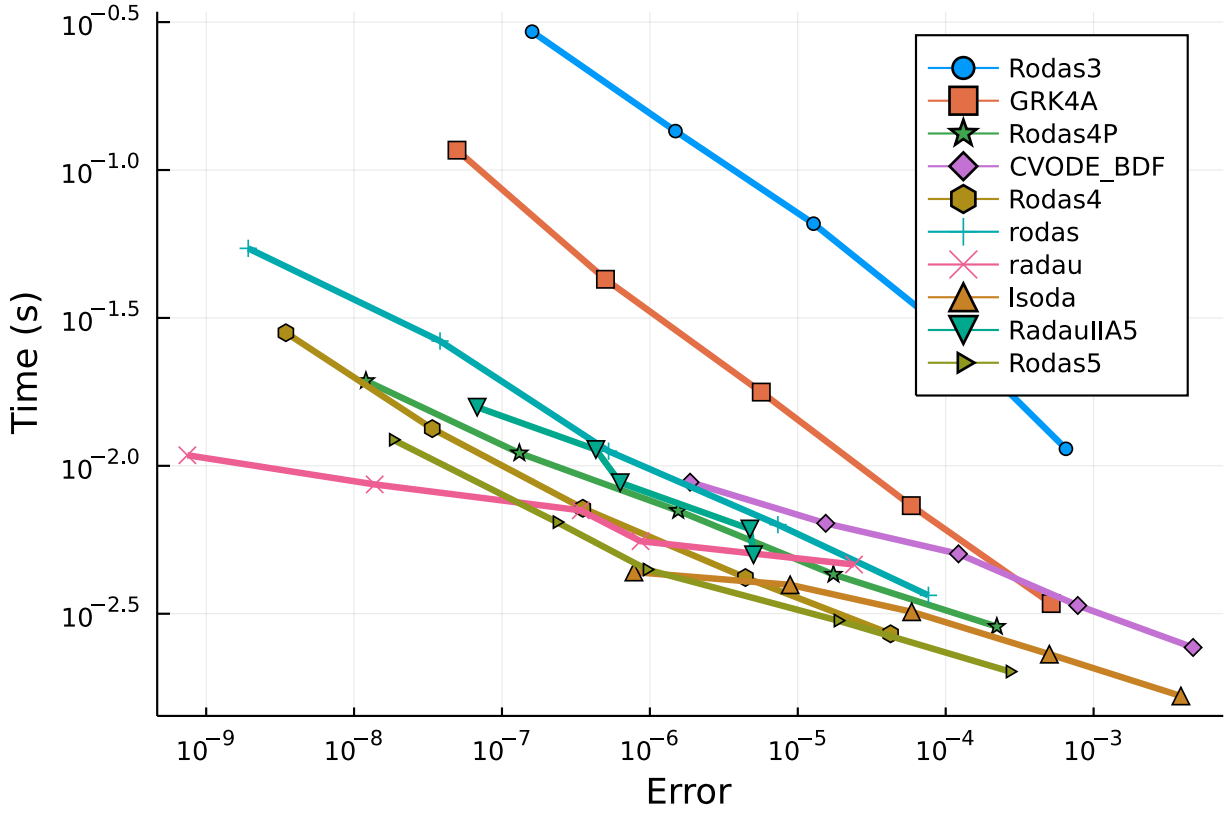
names=names,save_everystep=false,appxsol=test_sol,maxiters=Int(1e6),seconds=5)
plot(wp)
```




```
setups = [Dict(:alg=>Rodas3()),
          Dict(:alg=>CVODE_BDF()),
          Dict(:alg=>Rodas4()),
          Dict(:alg=>radau()),
          Dict(:alg=>Rodas5())]
wp = WorkPrecisionSet(prob,abstols,reltols,setups;
                      save_everystep=false,appxsol=test_sol,maxiters=Int(1e6),seconds=5)
plot(wp)
```

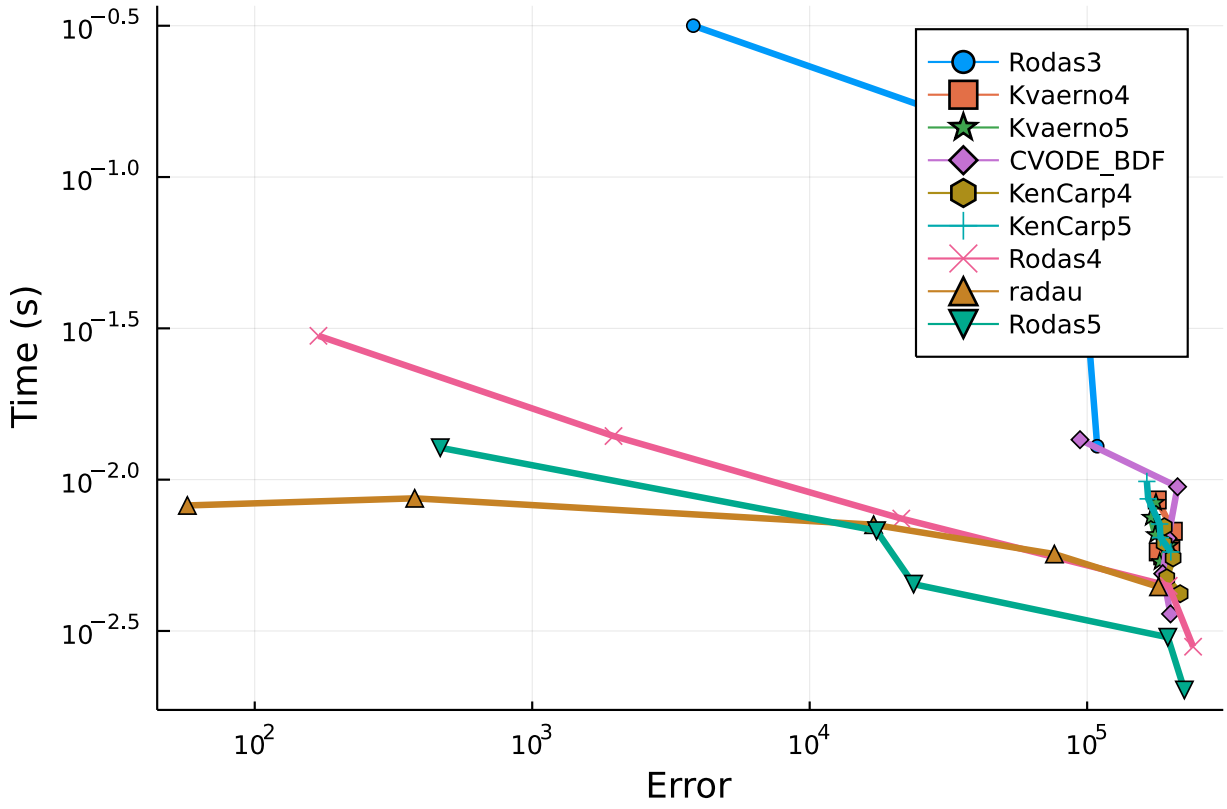



```
abstols = 1.0 ./ 10.0 .^ (7:11)
reltols = 1.0 ./ 10.0 .^ (4:8)
setups = [Dict(:alg=>Rodas3()),
          Dict(:alg=>GRK4A()),
          Dict(:alg=>Rodas4P()),
          Dict(:alg=>CVODE_BDF()),
          Dict(:alg=>Rodas4()),
          Dict(:alg=>rodas()),
          Dict(:alg=>radau()),
          Dict(:alg=>lsoda()),
          Dict(:alg=>RadauIIA5()),
          Dict(:alg=>Rodas5())]
wp = WorkPrecisionSet(prob,abstols,reltols,setups;error_estimate=:l2,
                      save_everystep=false,appxsol=test_sol,maxiters=Int(1e6),seconds=5)
plot(wp)
```

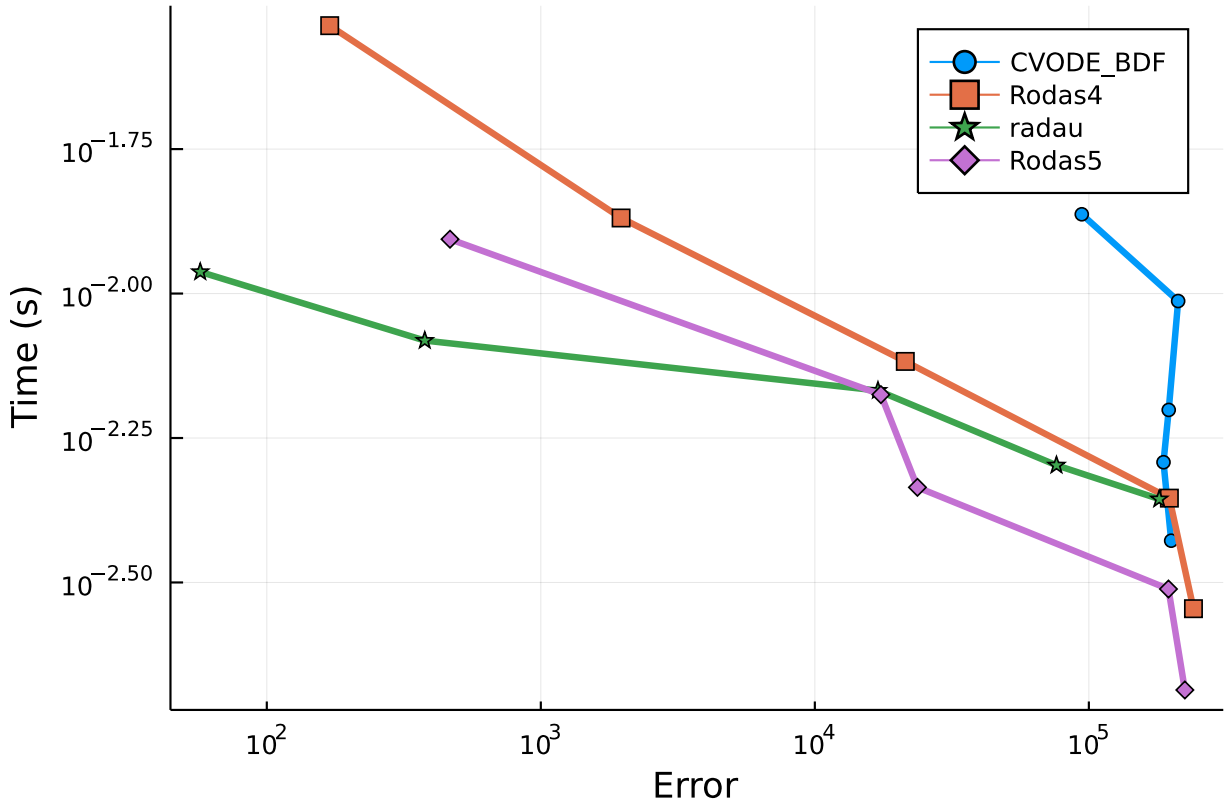



```
setups = [Dict(:alg=>Rodas3()),
          Dict(:alg=>Kvaerno4()),
          Dict(:alg=>Kvaerno5()),
          Dict(:alg=>CVODE_BDF()),
          Dict(:alg=>KenCarp4()),
          Dict(:alg=>KenCarp5()),
          Dict(:alg=>Rodas4()),
          Dict(:alg=>radau()),
          Dict(:alg=>Rodas5())]
names = ["Rodas3" "Kvaerno4" "Kvaerno5" "CVODE_BDF" "KenCarp4" "KenCarp5" "Rodas4"
"radau" "Rodas5"]
wp = WorkPrecisionSet(prob,abstols,reltols,setups;

names=names,appxsol=test_sol,maxiters=Int(1e6),error_estimate=:l2,seconds=5)
plot(wp)
```




```
setups = [Dict(:alg=>CVODE_BDF()),
          Dict(:alg=>Rodas4()),
          Dict(:alg=>radau()),
          Dict(:alg=>Rodas5())]
wp = WorkPrecisionSet(prob,abstols,reltols,setups;
                      appxsol=test_sol,maxiters=Int(1e6),error_estimate=:l2,seconds=5)
plot(wp)
```



The timeseries test is a little odd here because of the high peaks in the VanDerPol oscillator. At a certain accuracy, the steps try to resolve those peaks and so the error becomes higher.

While the higher order order Julia-based Rodas methods (`Rodas4` and `Rodas4P`) Rosenbrock methods are not viable at higher tolerances, they dominate for a large portion of this benchmark. When the tolerance gets low enough, `radau` adaptive high order (up to order 13) takes the lead.

0.2.2 Conclusion

`Rosenbrock23` and `Rodas3` do well when tolerances are higher. In most standard tolerances, `Rodas4` and `Rodas4P` do extremely well. Only when the tolerances get very low does `radau` do well. The Julia Rosenbrock methods vastly outperform their Fortran counterparts. `CVODE_BDF` is a top performer in the final timepoint errors with low accuracy, but take that with a grain of salt because the problem is periodic which means it's getting the spikes wrong but the low parts correct. `ARKODE` does poorly in these tests. `lsoda` does quite well in both low and high accuracy domains, but is never the top.

0.3 Appendix

These benchmarks are a part of the SciMLBenchmarks.jl repository, found at: https://github.com/SciML/
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","VanDerPol.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-ae0a
  JULIA_NUM_THREADS = 3
```

Package Information:

```
      Status `/var/lib/buildkite-agent/builds/rtx2070-gpuci1-julia-csail-mit-edu/julial
  [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
  [91a5bcdd] 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/julial
  [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
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[6a86dc24] FiniteDiff v2.8.0
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[59287772] Formatting v0.4.2
[f6369f11] ForwardDiff v0.10.18
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[5a33fad7] GeometricIntegratorsDiffEq v0.2.0
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[54ca160b] ODEInterface v0.5.0
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[429524aa] Optim v1.3.0
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[91a5bcdd] Plots v1.13.2
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[85a6dd25] PositiveFactorizations v0.2.4
[21216c6a] Preferences v1.2.2
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[fb686558] RandomExtensions v0.4.3
[e6cf234a] RandomNumbers v1.4.0
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[f2c3362d] RecursiveFactorization v0.1.12
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[ae029012] Requires v1.1.3
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[1bc83da4] SafeTestsets v0.0.1
[0bca4576] SciMLBase v1.13.2
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[6c6a2e73] Scratch v1.0.3
[efcf1570] Setfield v0.7.0
[992d4aef] Showoff v1.0.3
[699a6c99] SimpleTraits v0.9.3
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[47a9eef4] SparseDiffTools v1.13.2
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[a2a6695c] TreeViews v0.3.0
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[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
[34b6f7d7] FastTransforms_jll v0.4.1+0
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[559328eb] FriBidi_jll v1.0.5+6
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[d2c73de3] GR_jll v0.57.2+0
[78b55507] Gettext_jll v0.20.1+7
[f8c6e375] Git_jll v2.31.0+0
[7746bdde] Glib_jll v2.59.0+4
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[e9f186c6] Libffi_jll v3.2.1+4
[d4300ac3] Libgcrypt_jll v1.8.5+4
[7e76a0d4] Libglvnd_jll v1.3.0+3
[7add5ba3] Libgpg_error_jll v1.36.0+3
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[38a345b3] Libuuid_jll v2.34.0+7
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[c22f9ab0] Xorg_xcb_util_wm_jll v0.4.1+1
[35661453] Xorg_xkbcomp_jll v1.4.2+4
[33bec58e] Xorg_xkeyboard_config_jll v2.27.0+4
[c5fb5394] Xorg_xtrans_jll v1.4.0+3
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[6462fe0b] Sockets
[2f01184e] SparseArrays
[10745b16] Statistics
[4607b0f0] SuiteSparse
[fa267f1f] TOML
[a4e569a6] Tar
[8dfed614] Test
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[781609d7] GMP_jll
[deac9b47] LibCURL_jll
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[3a97d323] MPFR_jll
[c8ffd9c3] MbedTLS_jll
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[4536629a] OpenBLAS_jll
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[83775a58] Zlib_jll
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