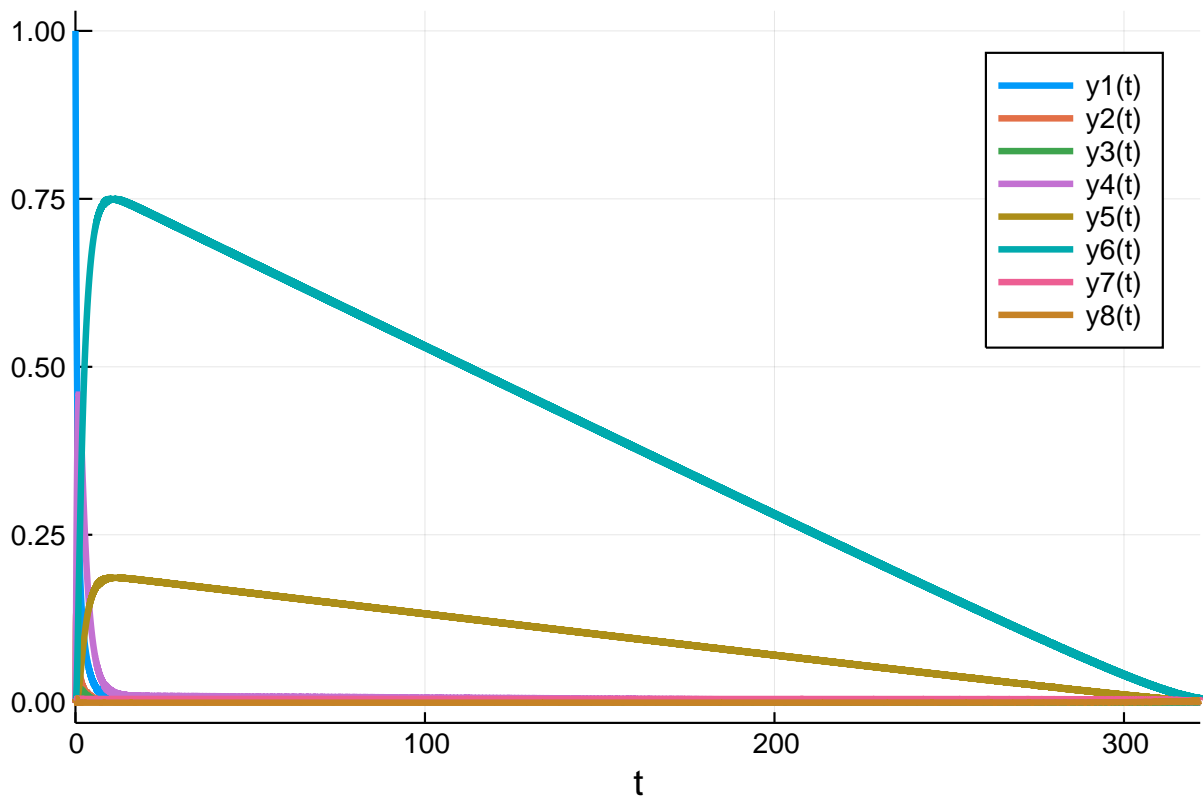


HIRES Work-Precision Diagrams

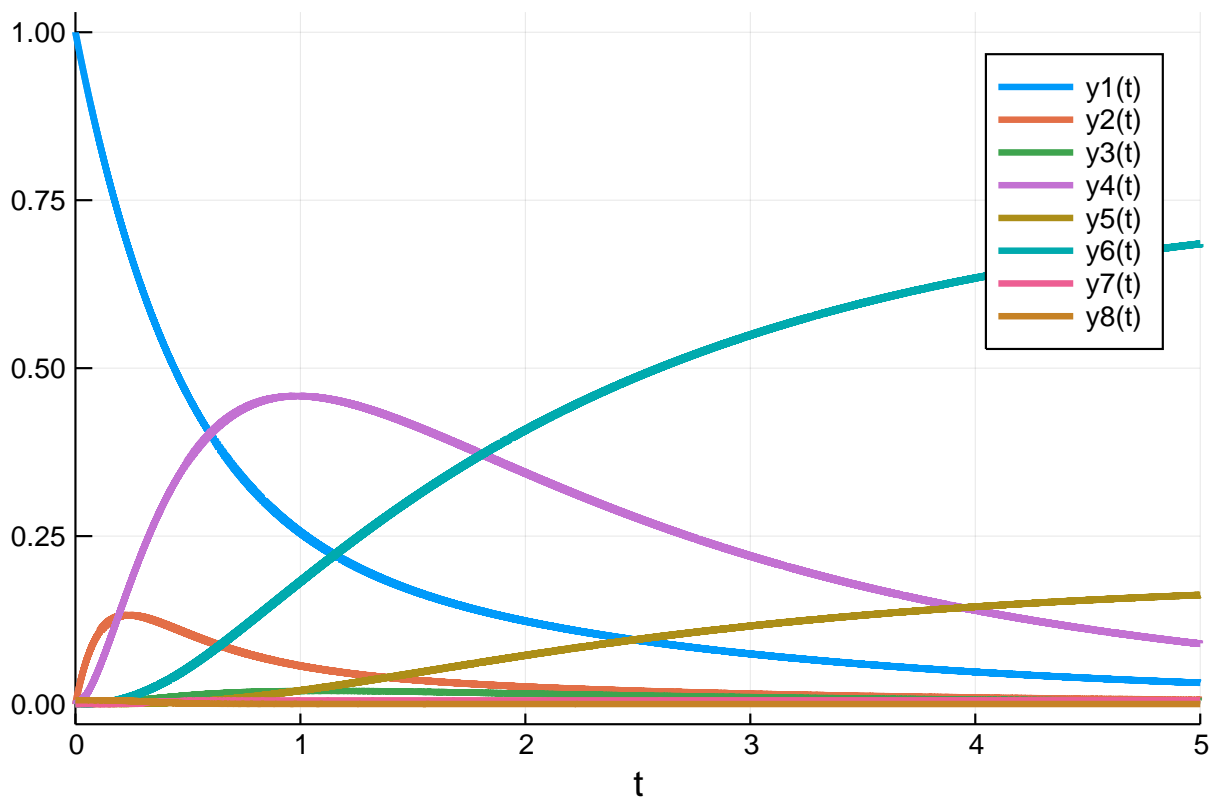
Chris Rackauckas

September 26, 2019

```
using OrdinaryDiffEq, ParameterizedFunctions, Plots, ODE, ODEInterfaceDiffEq, LSODA,  
    DiffEqDevTools, Sundials  
using LinearAlgebra  
LinearAlgebra.BLAS.set_num_threads(1)  
  
gr() #gr(fmt=:png)  
  
f = @ode_def Hires begin  
    dy1 = -1.71*y1 + 0.43*y2 + 8.32*y3 + 0.0007  
    dy2 = 1.71*y1 - 8.75*y2  
    dy3 = -10.03*y3 + 0.43*y4 + 0.035*y5  
    dy4 = 8.32*y2 + 1.71*y3 - 1.12*y4  
    dy5 = -1.745*y5 + 0.43*y6 + 0.43*y7  
    dy6 = -280.0*y6*y8 + 0.69*y4 + 1.71*y5 -  
          0.43*y6 + 0.69*y7  
    dy7 = 280.0*y6*y8 - 1.81*y7  
    dy8 = -280.0*y6*y8 + 1.81*y7  
end  
  
u0 = zeros(8)  
u0[1] = 1  
u0[8] = 0.0057  
prob = ODEProblem(f,u0,(0.0,321.8122))  
  
sol = solve(prob,Rodas5(), 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)
```



```
plot(sol, tspan=(0.0,5.0))
```



0.1 Omissions

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
```

The stabilized explicit methods are not stable enough to handle this problem well. While they don't diverge, they are really slow.

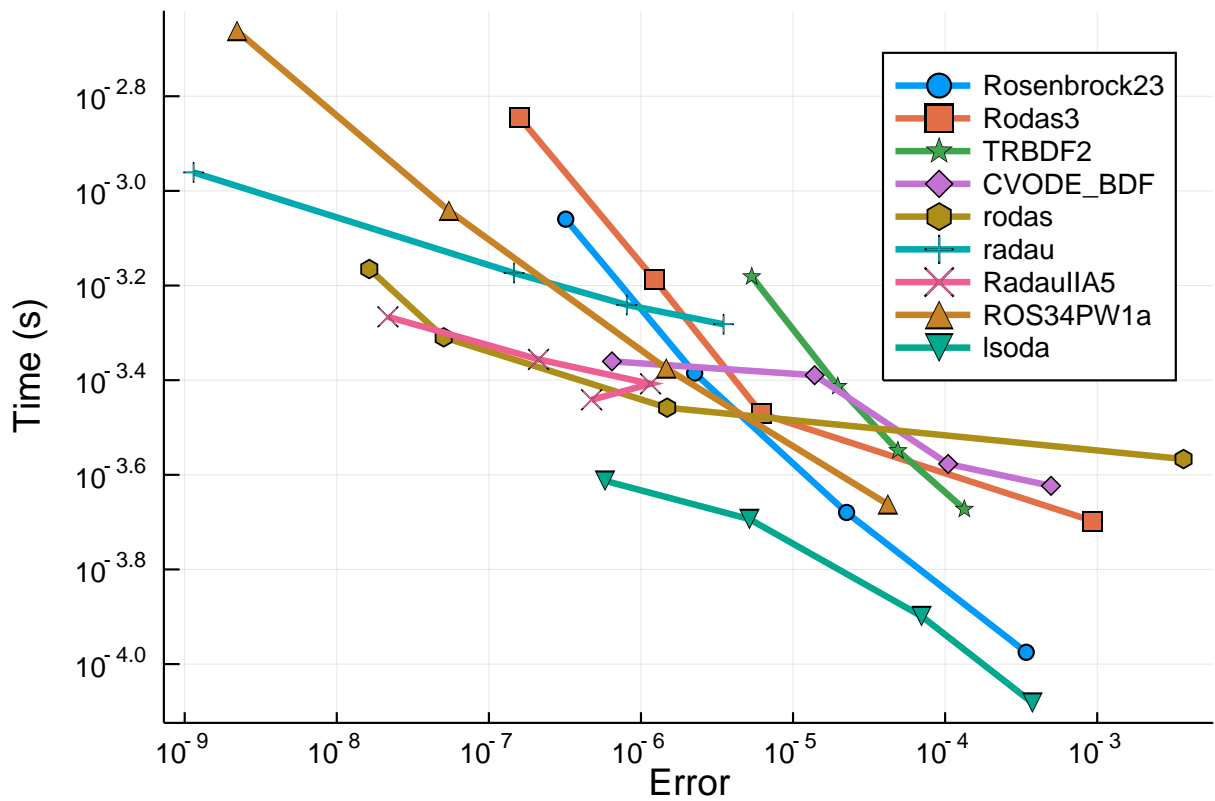
```
setups = [
#Dict(:alg=>ROCK2()),
#Dict(:alg=>ROCK4())
#Dict(:alg=>ESERK5())
]
```

0-element Array{Any,1}

0.2 High Tolerances

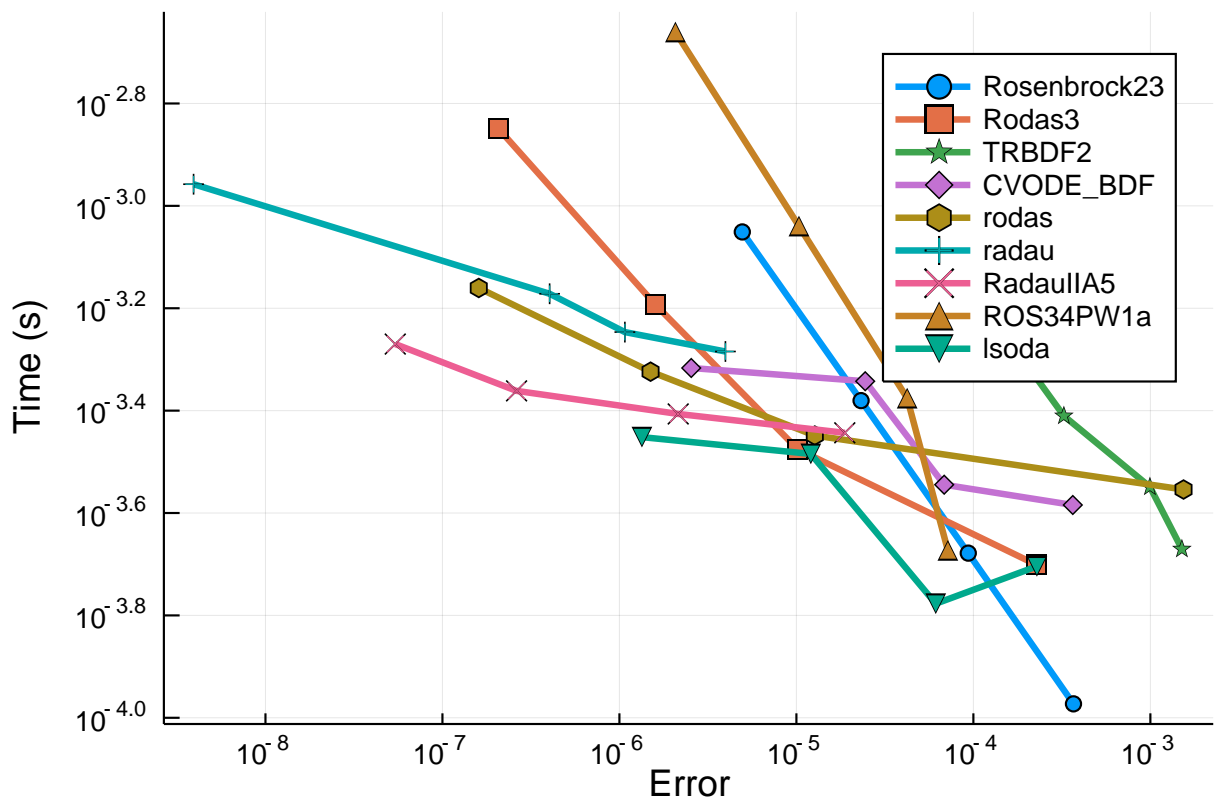
This is the speed when you just want the answer.

```
abstols = 1.0 ./ 10.0 .^ (5:8)
reltols = 1.0 ./ 10.0 .^ (1:4);
setups = [Dict(:alg=>Rosenbrock23()),
          Dict(:alg=>Rodas3()),
          Dict(:alg=>TRBDF2()),
          Dict(:alg=>CVODE_BDF()),
          Dict(:alg=>rodas()),
          Dict(:alg=>radau()),
          Dict(:alg=>RadauIIA5()),
          Dict(:alg=>ROS34PW1a()),
          Dict(:alg=>lsoda()),
        ]
wp = WorkPrecisionSet(prob,abstols,reltols,setups;
                      save_everystep=false,appxsol=test_sol,maxiters=Int(1e5),numruns=10)
plot(wp)
```



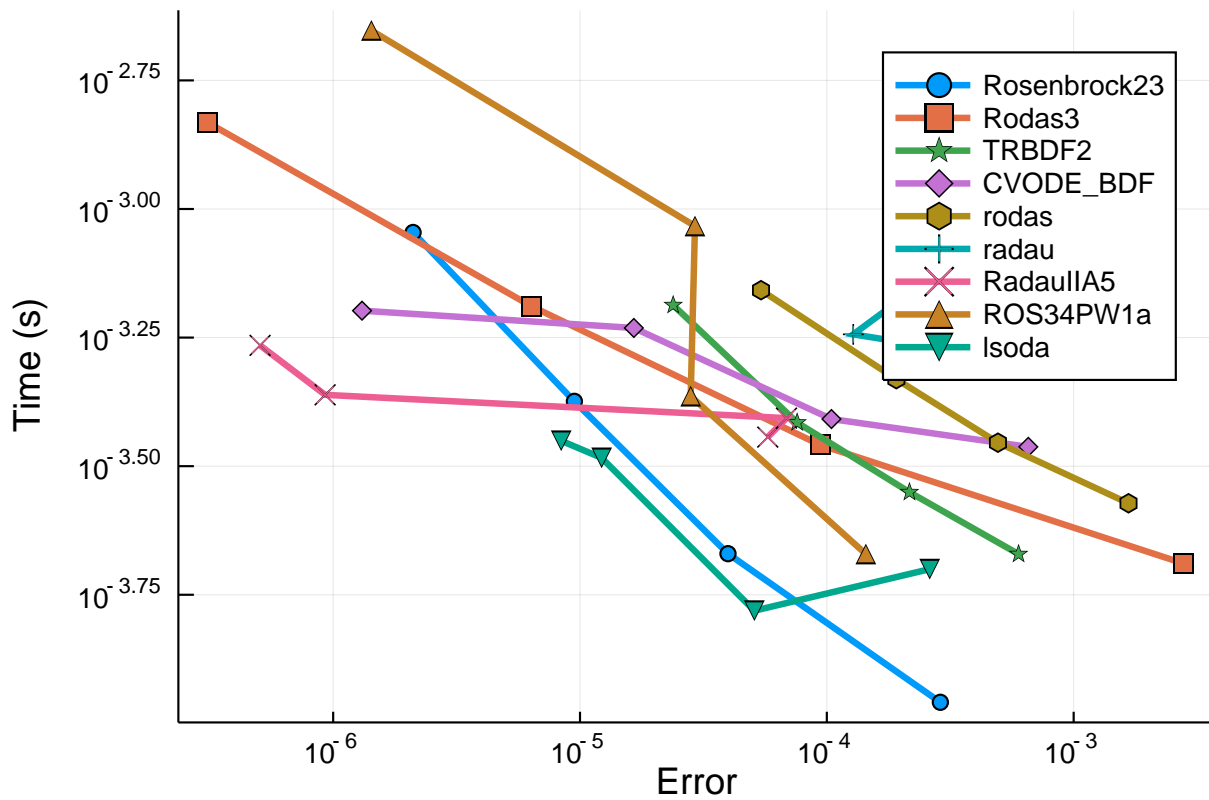
```
wp = WorkPrecisionSet(prob, abstols, reltols, setups; dense = false, verbose=false,
    appxsol=test_sol, maxiters=Int(1e5), error_estimate=:l2)
```

```
plot(wp)
```



```
wp = WorkPrecisionSet(prob, abstols, reltols, setups;
    appxsol=test_sol, maxiters=Int(1e5), error_estimate=:L2)
```

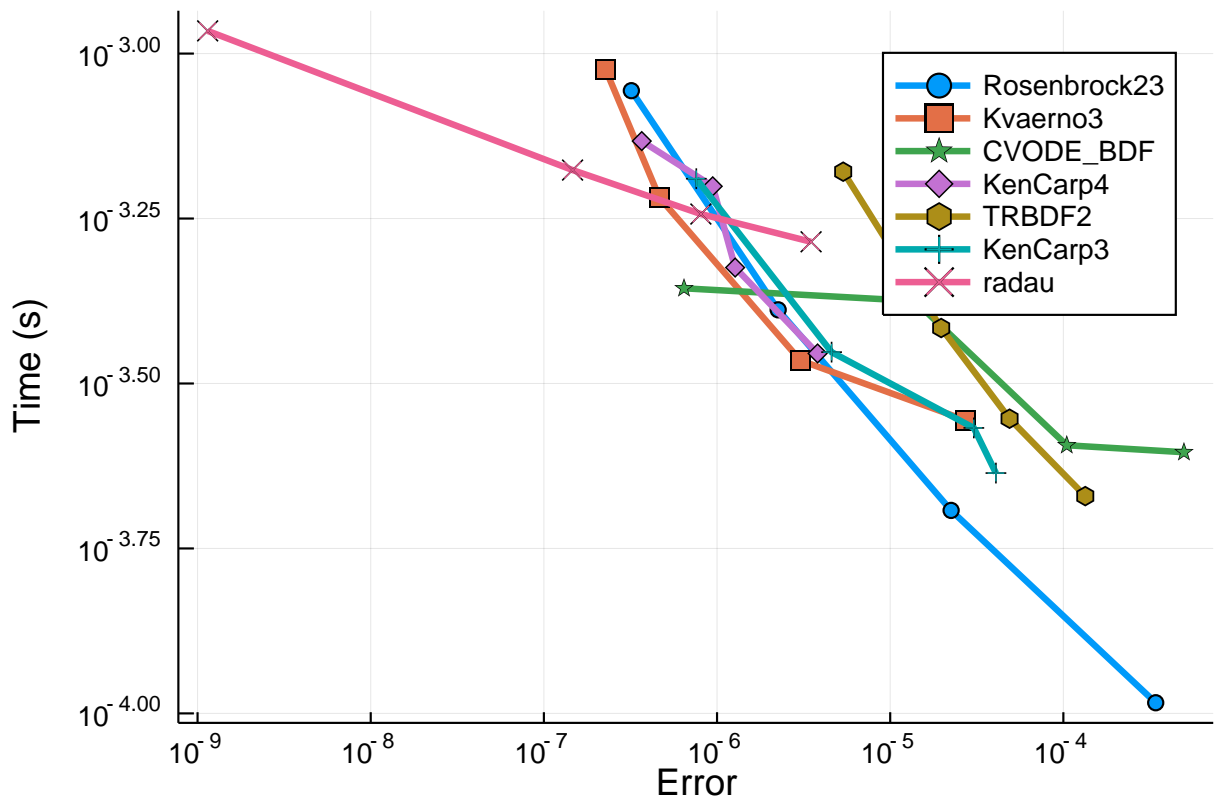
plot(wp)



```

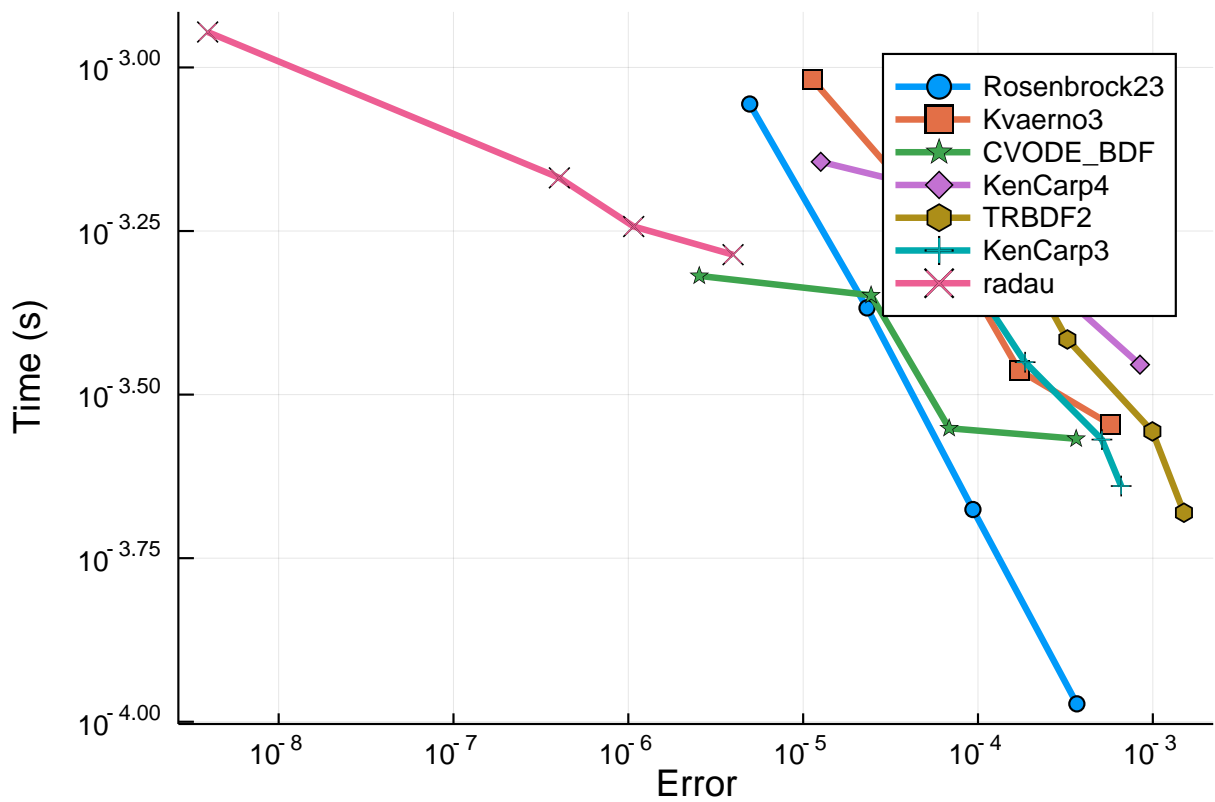
setups = [Dict(:alg=>Rosenbrock23()),
          Dict(:alg=>Kvaerno3()),
          Dict(:alg=>CVODE_BDF()),
          Dict(:alg=>KenCarp4()),
          Dict(:alg=>TRBDF2()),
          Dict(:alg=>KenCarp3()),
          # Dict(:alg=>SDIRK2()), # Removed because it's bad
          Dict(:alg=>radau())]
wp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

```



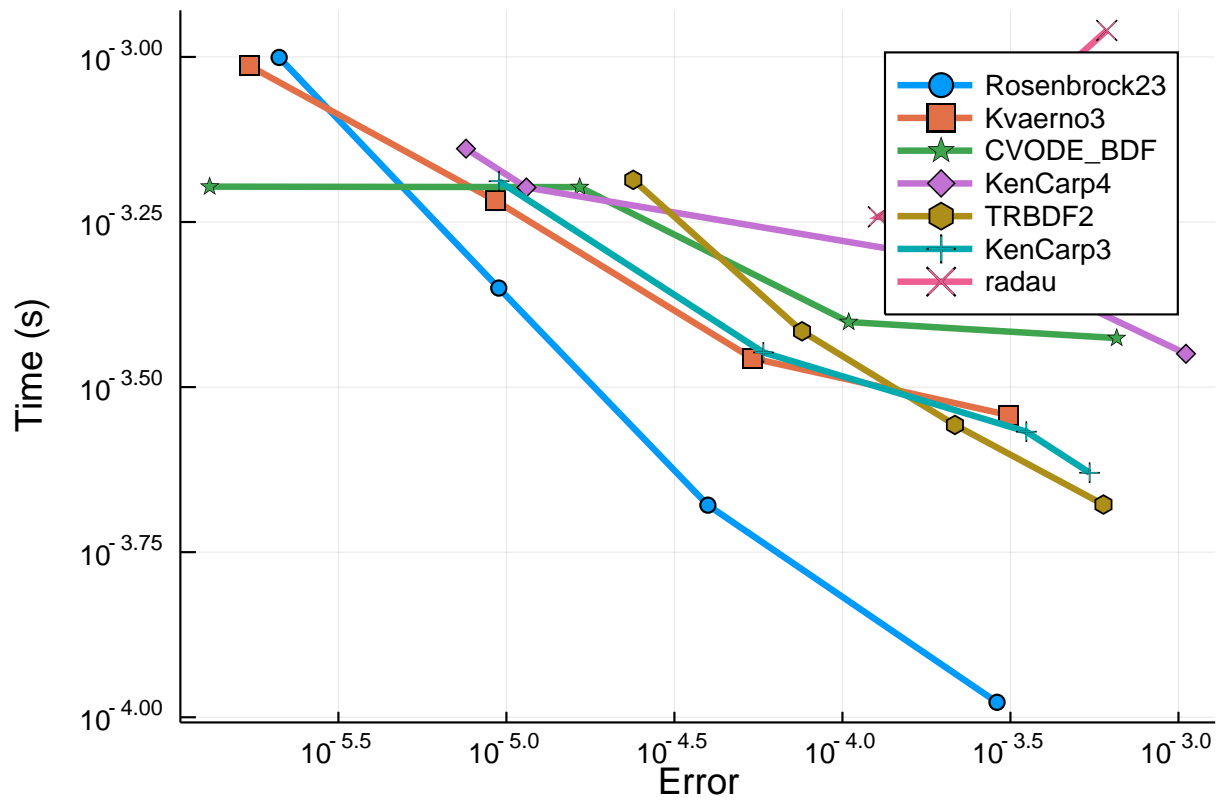
```
wp = WorkPrecisionSet(prob, abstols, reltols, setups; dense = false, verbose=false,
    appxsol=test_sol, maxiters=Int(1e5), error_estimate=:l2)
```

```
plot(wp)
```



```
wp = WorkPrecisionSet(prob, abstols, reltols, setups;
    appxsol=test_sol, maxiters=Int(1e5), error_estimate=:L2)
```

```
plot(wp)
```



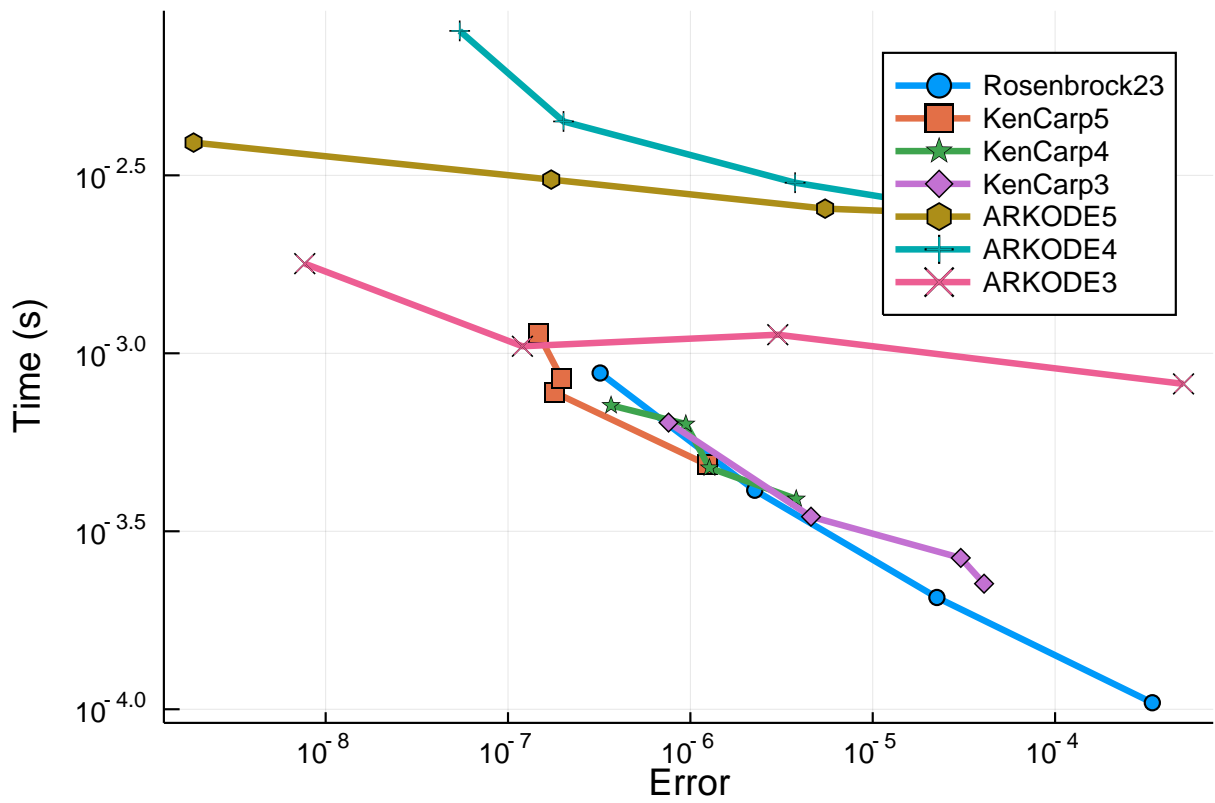
```

setups = [Dict(:alg=>Rosenbrock23()),
           Dict(:alg=>KenCarp5()),
           Dict(:alg=>KenCarp4()),
           Dict(:alg=>KenCarp3()),
           Dict(:alg=>ARKODE(order=5)),
           Dict(:alg=>ARKODE()),
           Dict(:alg=>ARKODE(order=3))]

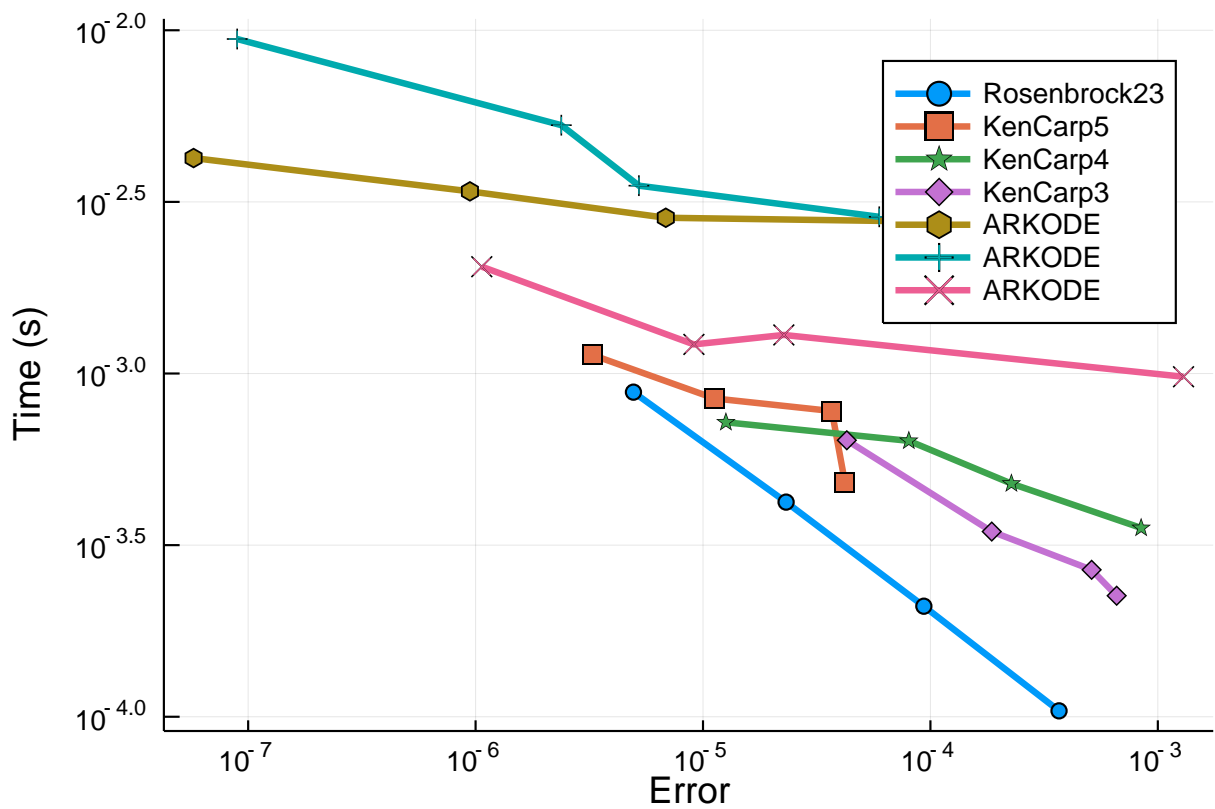
names = ["Rosenbrock23" "KenCarp5" "KenCarp4" "KenCarp3" "ARKODE5" "ARKODE4" "ARKODE3"]
wp = WorkPrecisionSet(prob, abstols, reltols, setups;

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

```



```
wp = WorkPrecisionSet(prob, abstols, reltols, setups; dense = false, verbose = false,
    appxsol = test_sol, maxiters = Int(1e5), error_estimate = :l2)
plot(wp)
```



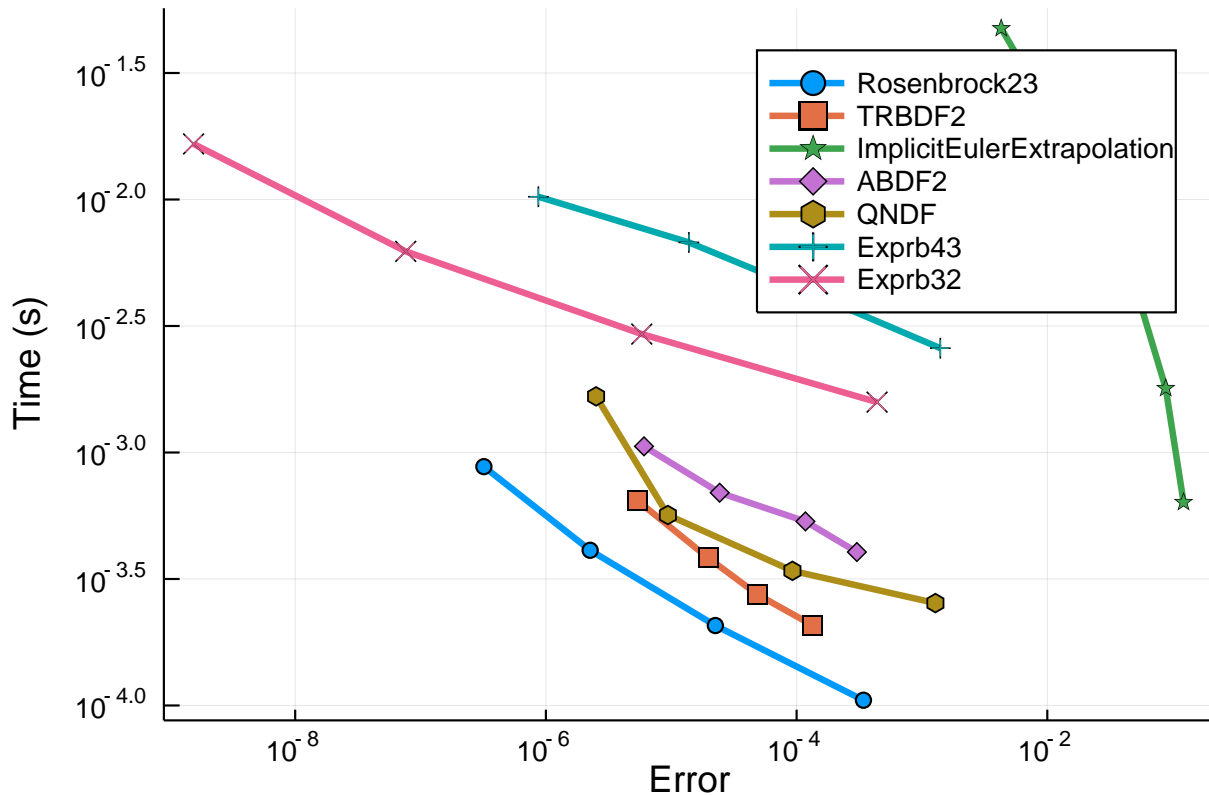
```
setups = [Dict(:alg => Rosenbrock23()),
    Dict(:alg => TRBDF2()),
```



```

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

```



0.2.1 Low Tolerances

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

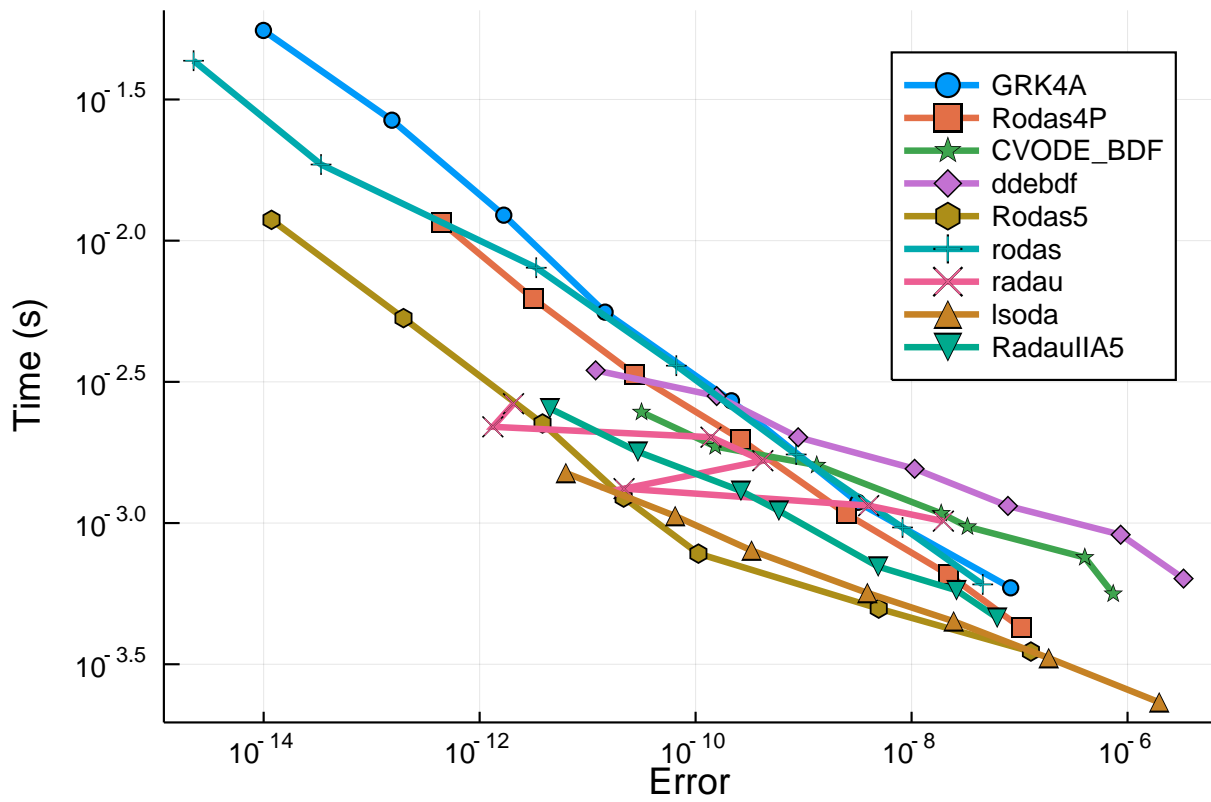
```

abstols = 1.0 ./ 10.0 .^ (7:13)
reltols = 1.0 ./ 10.0 .^ (4:10)

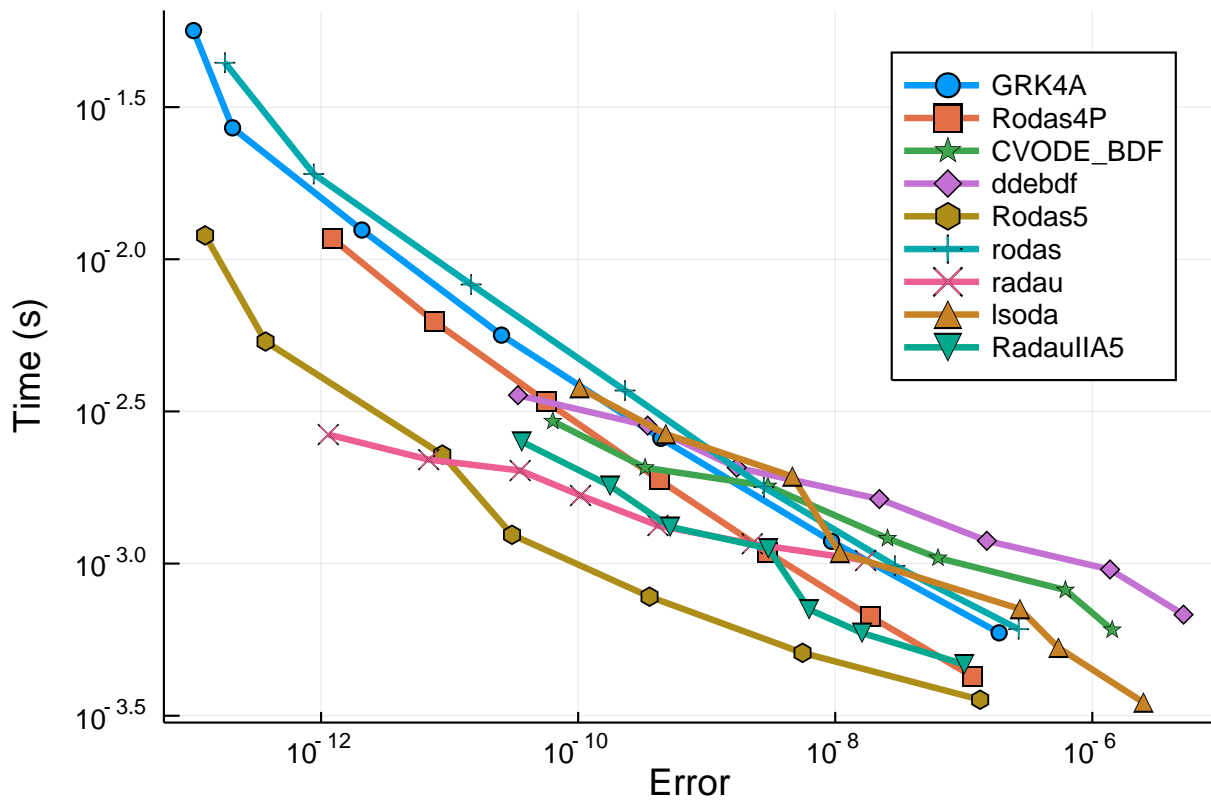
setups = [Dict(:alg=>GRK4A()),
    Dict(:alg=>Rodas4P()),
    Dict(:alg=>CVODE_BDF()),
    Dict(:alg=>ddebdf()),
    Dict(:alg=>Rodas5()),
    Dict(:alg=>rodas()),
    Dict(:alg=>radau()),
    Dict(:alg=>lsoda()),
    Dict(:alg=>RadauIIA5()),
]
wp = WorkPrecisionSet(prob, abstols, reltols, setups;
    save_everystep=false, appxsol=test_sol, maxiters=Int(1e5))

```

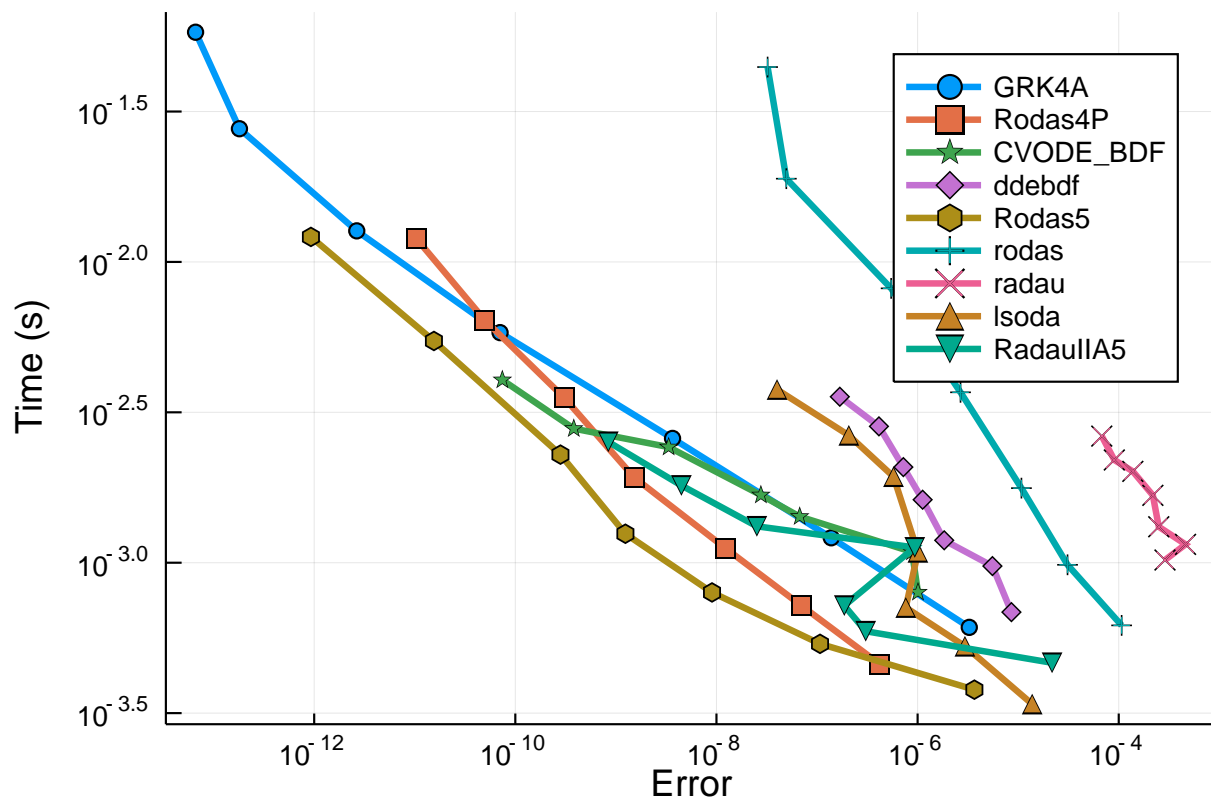
plot(wp)



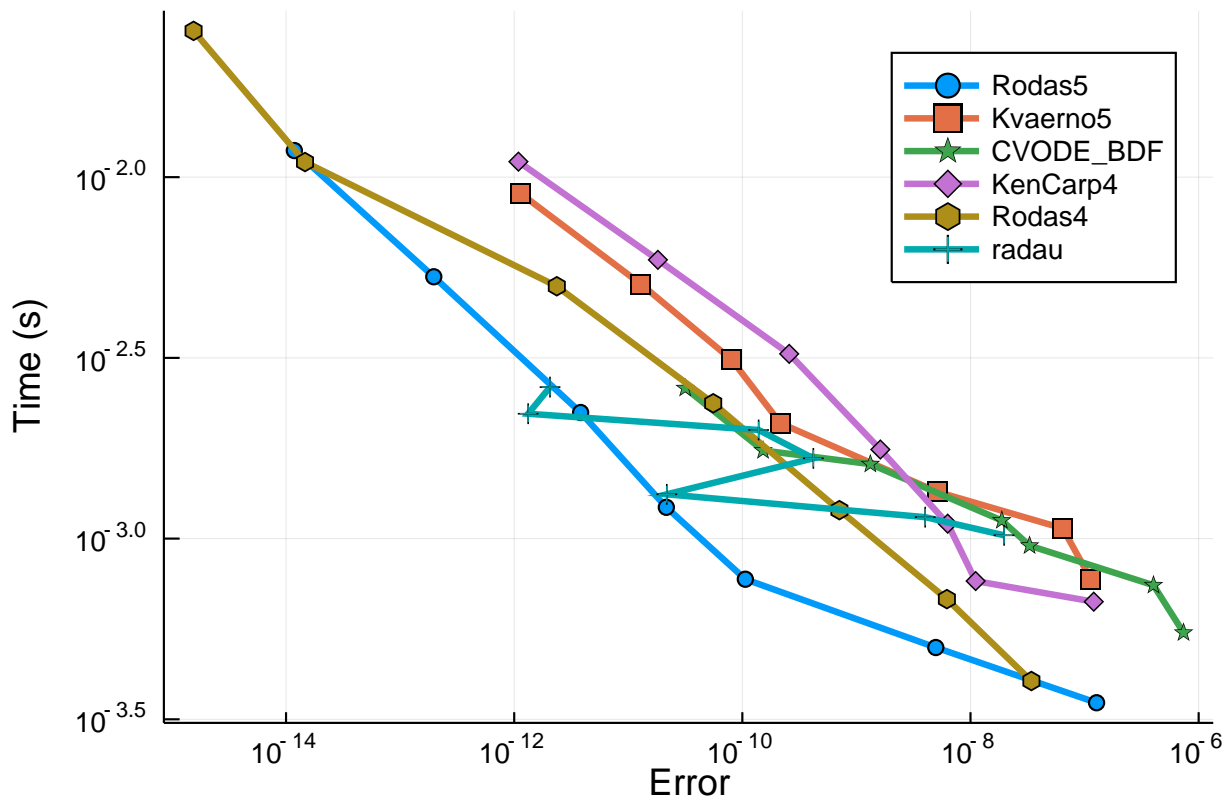
```
wp = WorkPrecisionSet(prob, abstols, reltols, setups; verbose=false,
    dense=false, appxsol=test_sol, maxiters=Int(1e5), error_estimate=:l2)
plot(wp)
```



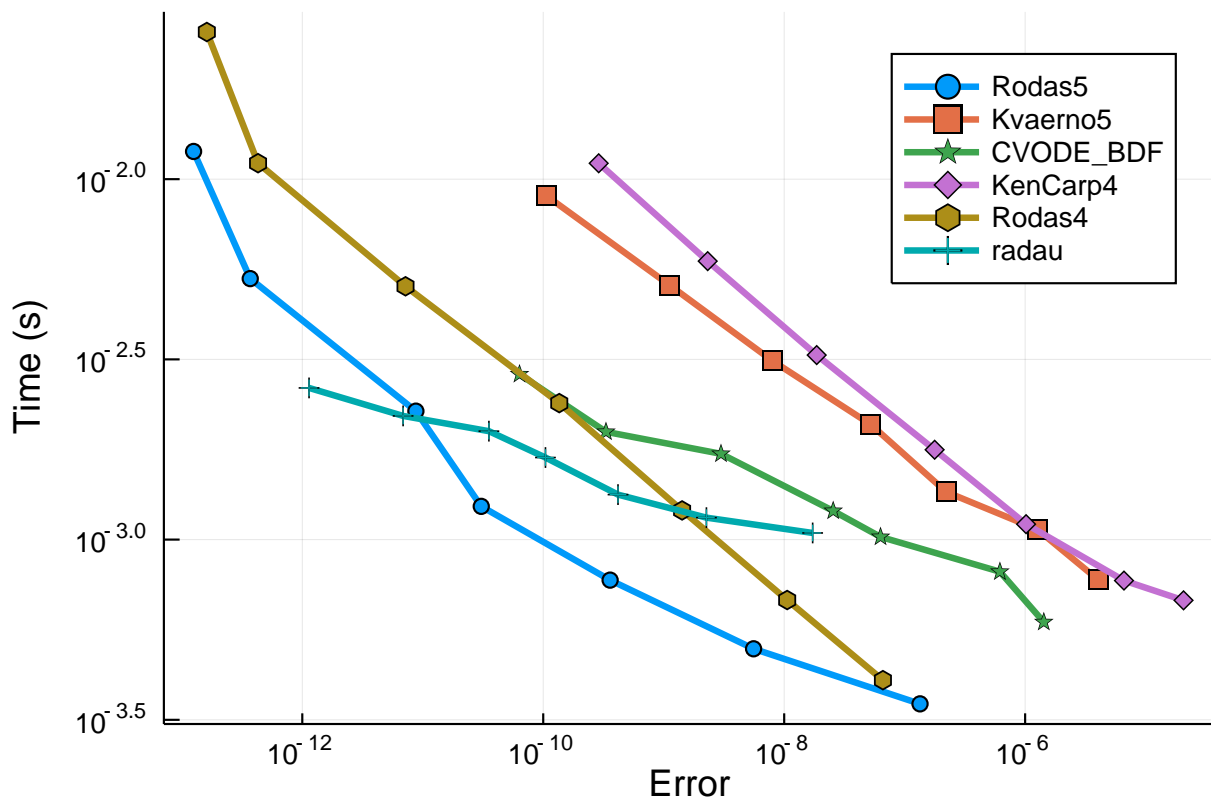
```
wp = WorkPrecisionSet(prob, abstols, reltols, setups;
    appxsol=test_sol, maxiters=Int(1e5), error_estimate=:L2)
plot(wp)
```



```
setups = [
    Dict(:alg=>Rodas5()),
    Dict(:alg=>Kvaerno5()),
    Dict(:alg=>CVODE_BDF()),
    Dict(:alg=>KenCarp4()),
    Dict(:alg=>Rodas4()),
    Dict(:alg=>radau())]
wp = WorkPrecisionSet(prob, abstols, reltols, setups;
    save_everystep=false, appxsol=test_sol, maxiters=Int(1e5))
plot(wp)
```

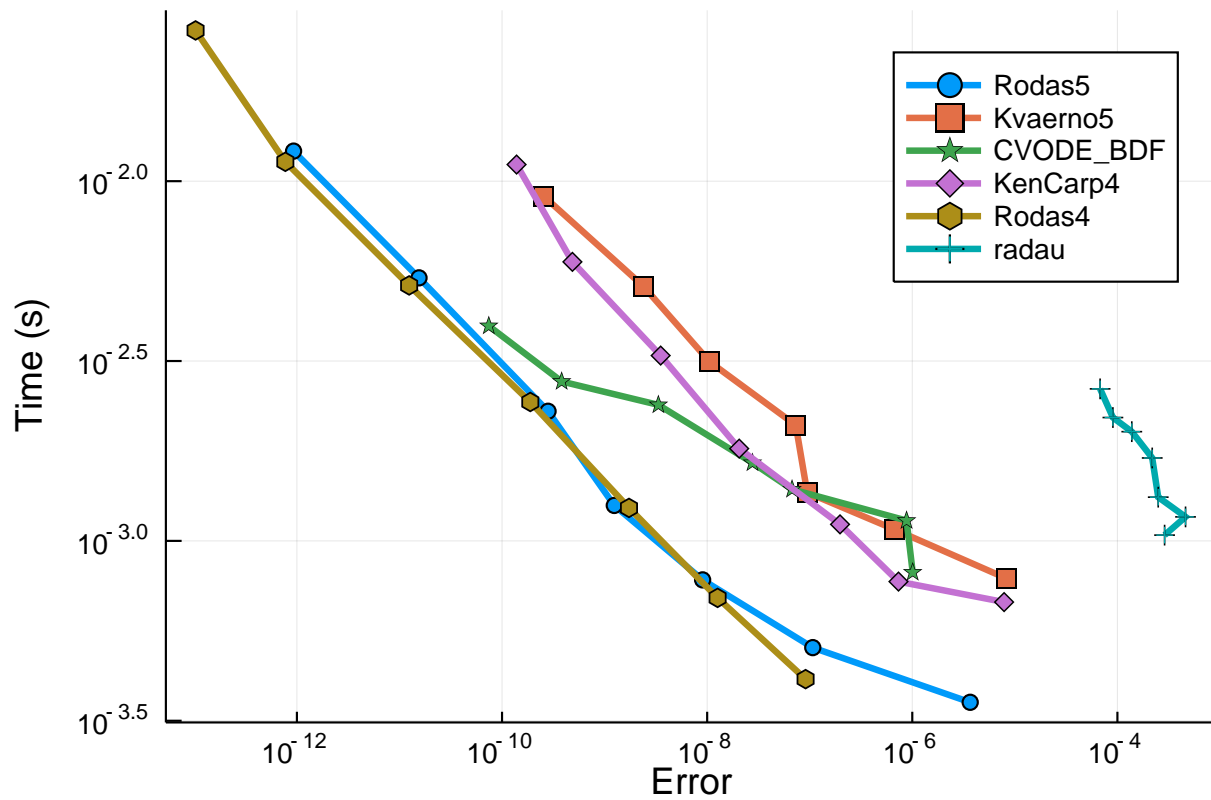


```
wp = WorkPrecisionSet(prob, abstols, reltols, setups; verbose=false,
    dense=false, appxsol=test_sol, maxiters=Int(1e5), error_estimate=:l2)
plot(wp)
```



```
wp = WorkPrecisionSet(prob, abstols, reltols, setups;
    appxsol=test_sol, maxiters=Int(1e5), error_estimate=:L2)
```

```
plot(wp)
```



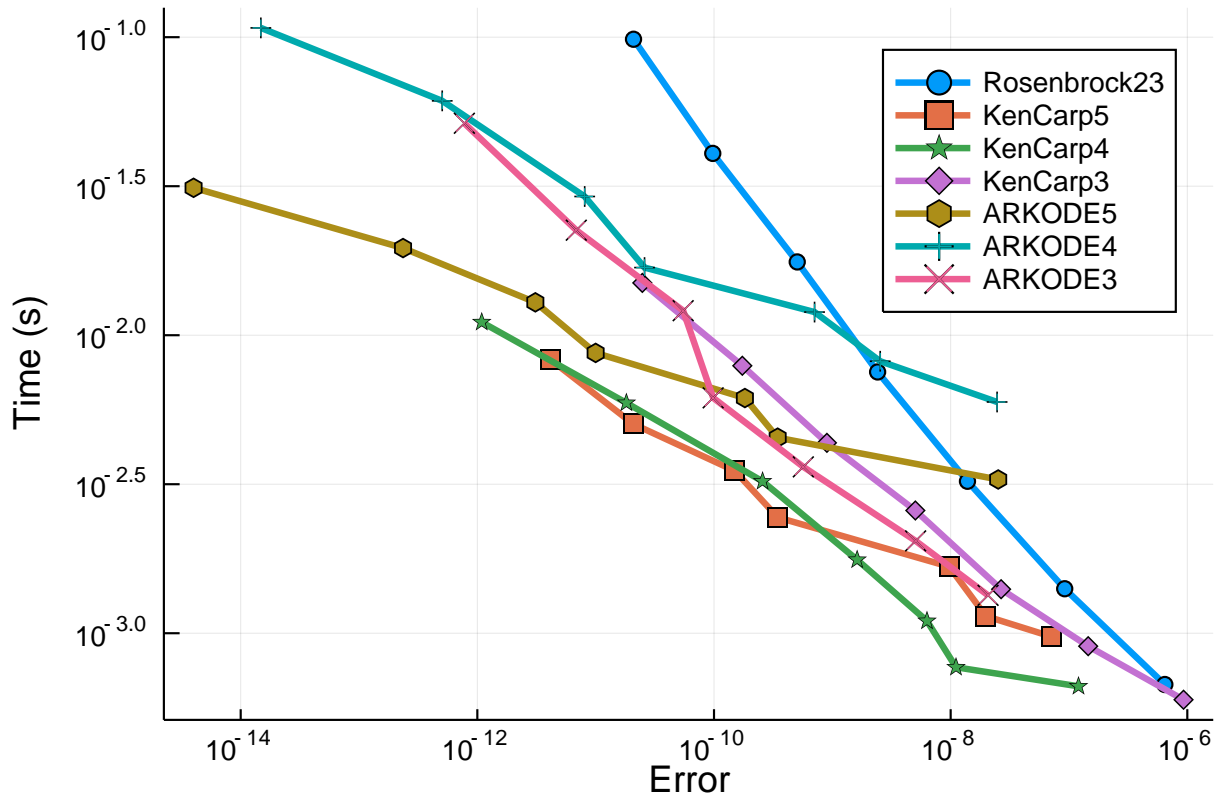
```

setups = [Dict(:alg=>Rosenbrock23()),
          Dict(:alg=>KenCarp5()),
          Dict(:alg=>KenCarp4()),
          Dict(:alg=>KenCarp3()),
          Dict(:alg=>ARKODE(order=5)),
          Dict(:alg=>ARKODE()),
          Dict(:alg=>ARKODE(order=3))]

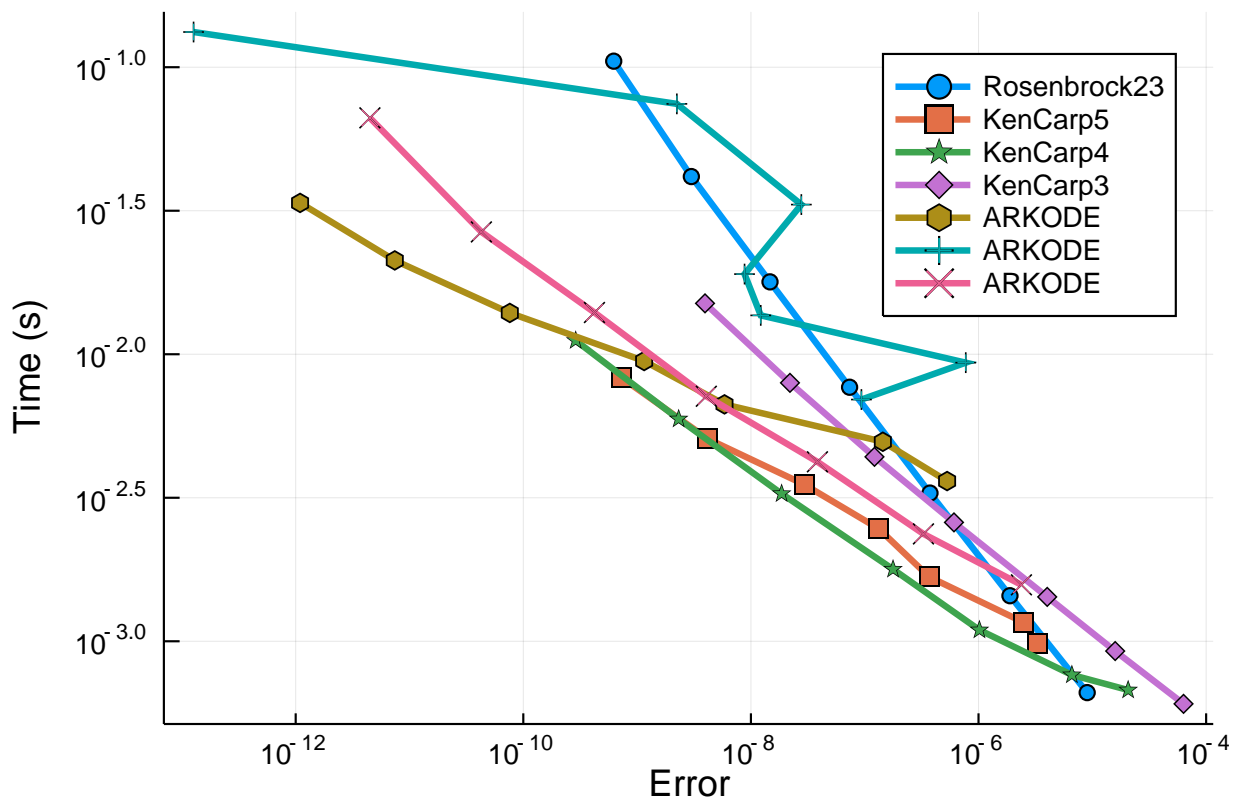
names = ["Rosenbrock23" "KenCarp5" "KenCarp4" "KenCarp3" "ARKODE5" "ARKODE4" "ARKODE3"]
wp = WorkPrecisionSet(prob, abstols, reltols, setups;

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

```



```
wp = WorkPrecisionSet(prob, abstols, reltols, setups; verbose=false,
    dense=false, appxsol=test_sol, maxiters=Int(1e5), error_estimate=:l2)
plot(wp)
```



The following algorithms were removed since they failed.

```

#setups = [#Dict(:alg=>Hairer4()),
           #Dict(:alg=>Hairer42()),
           #Dict(:alg=>Rodas3()),
           #Dict(:alg=>Kvaerno4()),
           #Dict(:alg=>KenCarp5()),
           #Dict(:alg=>Cash4())
#]
#wp = WorkPrecisionSet(prob, abstols, reltols, setups;
# save_everystep=false, appxsol=test_sol, maxiters=Int(1e5))
#plot(wp)

```

0.2.2 Conclusion

At high tolerances, `Rosenbrock23` and `lsoda` hits the the error estimates and are fast. At lower tolerances and normal user tolerances, `Rodas5` is extremely fast. When you get down to `reltol=1e-10` `radau` begins to become as efficient as `Rodas4`, and it continues to do well below that.

```

using DiffEqBenchmarks
DiffEqBenchmarks.bench_footer(WEAVE_ARGS[:folder], WEAVE_ARGS[:file])

```

0.3 Appendix

These benchmarks are a part of the `DiffEqBenchmarks.jl` repository, found at: <https://github.com/JuliaDiffEq/DiffEqBenchmarks.jl>

To locally run this tutorial, do the following commands:

```

using DiffEqBenchmarks
DiffEqBenchmarks.weave_file("StiffODE", "Hires.jmd")

```

Computer Information:

```

Julia Version 1.2.0
Commit c6da87ff4b (2019-08-20 00:03 UTC)
Platform Info:
  OS: Linux (x86_64-pc-linux-gnu)
  CPU: Intel(R) Xeon(R) CPU E5-2680 v4 @ 2.40GHz
  WORD_SIZE: 64
  LIBM: libopenlibm
  LLVM: libLLVM-6.0.1 (ORCJIT, haswell)
Environment:
  JULIA_NUM_THREADS = 16

```

Package Information:

```

Status: `~/home/crackauckas/.julia/dev/DiffEqBenchmarks/Project.toml`
[a134a8b2-14d6-55f6-9291-3336d3ab0209] BlackBoxOptim 0.5.0
[f3b72e0c-5b89-59e1-b016-84e28bfd966d] DiffEqDevTools 2.15.0

```

[1130ab10-4a5a-5621-a13d-e4788d82bd4c] DiffEqParamEstim 1.8.0
 [a077e3f3-b75c-5d7f-a0c6-6bc4c8ec64a9] DiffEqProblemLibrary 4.5.1
 [ef61062a-5684-51dc-bb67-a0fcdec5c97d] DiffEqUncertainty 1.2.0
 [7073ff75-c697-5162-941a-fcdaad2a7d2a] IJulia 1.20.0
 [7f56f5a3-f504-529b-bc02-0b1fe5e64312] LSODA 0.6.1
 [76087f3c-5699-56af-9a33-bf431cd00edd] NLOpt 0.5.1
 [c030b06c-0b6d-57c2-b091-7029874bd033] ODE 2.5.0
 [54ca160b-1b9f-5127-a996-1867f4bc2a2c] ODEInterface 0.4.6
 [09606e27-ecf5-54fc-bb29-004bd9f985bf] ODEInterfaceDiffEq 3.4.0
 [1dea7af3-3e70-54e6-95c3-0bf5283fa5ed] OrdinaryDiffEq 5.17.1
 [65888b18-ceab-5e60-b2b9-181511a3b968] ParameterizedFunctions 4.2.1
 [91a5bcd-d5d7-5caf-9e0b-520d859cae80] Plots 0.26.3
 [c3572dad-4567-51f8-b174-8c6c989267f4] Sundials 3.7.0
 [44d3d7a6-8a23-5bf8-98c5-b353f8df5ec9] Weave 0.9.1
 [b77e0a4c-d291-57a0-90e8-8db25a27a240] InteractiveUtils
 [d6f4376e-aef5-505a-96c1-9c027394607a] Markdown
 [44cfe95a-1eb2-52ea-b672-e2afdf69b78f] Pkg
 [9a3f8284-a2c9-5f02-9a11-845980a1fd5c] Random