POLLU Work-Precision Diagrams

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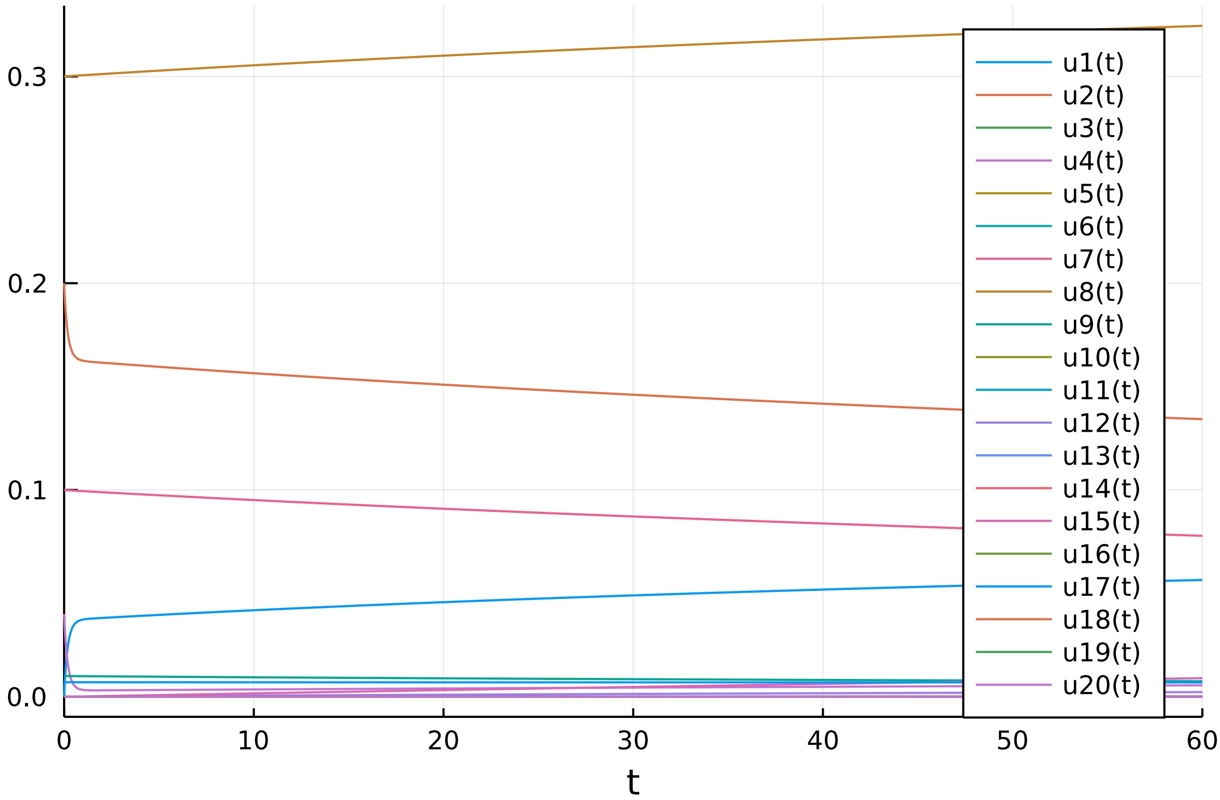
```julia
using OrdinaryDiffEq, DiffEqDevTools, Sundials, ParameterizedFunctions, Plots, ODE,
ODEInterfaceDiffEq, LSODA
gr() # gr(fmt=:png)
using LinearAlgebra

const k1=.35e0
const k2=.266e2
const k3=.123e5
const k4=.86e-3
const k5=.82e-3
const k6=.15e5
const k7=.13e-3
const k8=.24e5
const k9=.165e5
const k10=.9e4
const k11=.22e-1
const k12=.12e5
const k13=.188e1
const k14=.163e5
const k15=.48e7
const k16=.35e-3
const k17=.175e-1
const k18=.1e9
const k19=.444e12
const k20=.124e4
const k21=.21e1
const k22=.578e1
const k23=.474e-1
const k24=.178e4
const k25=.312e1

function f(dy,y,p,t)
 r1  = k1 *y[1]
 r2  = k2 *y[2]*y[4]
 r3  = k3 *y[5]*y[2]
 r4  = k4 *y[7]
 r5  = k5 *y[7]
 r6  = k6 *y[7]*y[6]
 r7  = k7 *y[9]
 r8  = k8 *y[9]*y[6]
 r9  = k9 *y[11]*y[2]
 r10 = k10*y[11]*y[1]
 r11 = k11*y[13]
 r12 = k12*y[10]*y[2]
 r13 = k13*y[14]
```

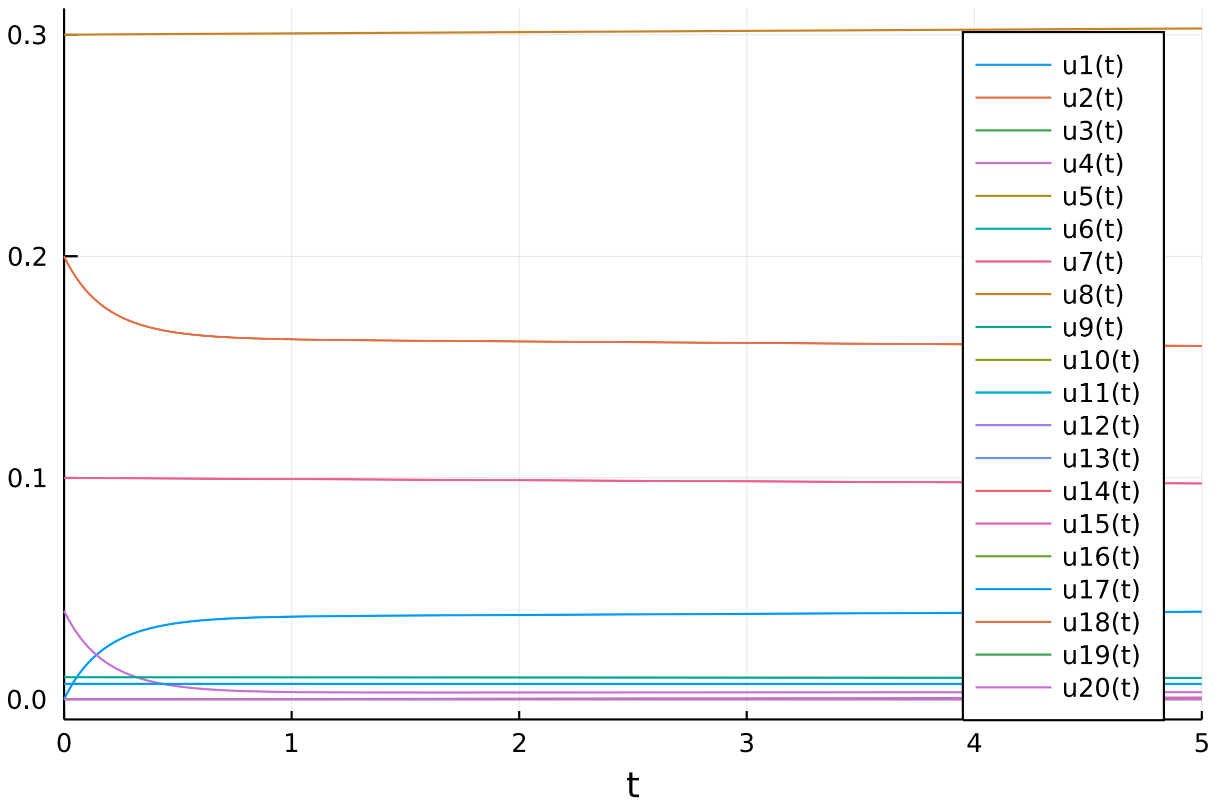
```julia
 r14 = k14*y[1]*y[6]
 r15 = k15*y[3]
 r16 = k16*y[4]
 r17 = k17*y[4]
 r18 = k18*y[16]
 r19 = k19*y[16]
 r20 = k20*y[17]*y[6]
 r21 = k21*y[19]
 r22 = k22*y[19]
 r23 = k23*y[1]*y[4]
 r24 = k24*y[19]*y[1]
 r25 = k25*y[20]

 dy[1]  = -r1-r10-r14-r23-r24+
          r2+r3+r9+r11+r12+r22+r25
 dy[2]  = -r2-r3-r9-r12+r1+r21
 dy[3]  = -r15+r1+r17+r19+r22
 dy[4]  = -r2-r16-r17-r23+r15
 dy[5]  = -r3+r4+r4+r6+r7+r13+r20
 dy[6]  = -r6-r8-r14-r20+r3+r18+r18
 dy[7]  = -r4-r5-r6+r13
 dy[8]  = r4+r5+r6+r7
 dy[9]  = -r7-r8
 dy[10] = -r12+r7+r9
 dy[11] = -r9-r10+r8+r11
 dy[12] = r9
 dy[13] = -r11+r10
 dy[14] = -r13+r12
 dy[15] = r14
 dy[16] = -r18-r19+r16
 dy[17] = -r20
 dy[18] = r20
 dy[19] = -r21-r22-r24+r23+r25
 dy[20] = -r25+r24
end

function fjac(J,y,p,t)
      J .= 0.0
      J[1,1]   = -k1-k10*y[11]-k14*y[6]-k23*y[4]-k24*y[19]
      J[1,11]  = -k10*y[1]+k9*y[2]
      J[1,6]   = -k14*y[1]
      J[1,4]   = -k23*y[1]+k2*y[2]
      J[1,19]  = -k24*y[1]+k22
      J[1,2]   = k2*y[4]+k9*y[11]+k3*y[5]+k12*y[10]
      J[1,13]  = k11
      J[1,20]  = k25
      J[1,5]   = k3*y[2]
      J[1,10]  = k12*y[2]

      J[2,4]   = -k2*y[2]
      J[2,5]   = -k3*y[2]
      J[2,11]  = -k9*y[2]
      J[2,10]  = -k12*y[2]
      J[2,19]  = k21
      J[2,1]   = k1
      J[2,2]   = -k2*y[4]-k3*y[5]-k9*y[11]-k12*y[10]

      J[3,1]   = k1
      J[3,4]   = k17
```

```
J[3,16]  = k19
J[3,19]  = k22
J[3,3]   = -k15

J[4,4]   = -k2*y[2]-k16-k17-k23*y[1]
J[4,2]   = -k2*y[4]
J[4,1]   = -k23*y[4]
J[4,3]   = k15

J[5,5]   = -k3*y[2]
J[5,2]   = -k3*y[5]
J[5,7]   = 2k4+k6*y[6]
J[5,6]   = k6*y[7]+k20*y[17]
J[5,9]   = k7
J[5,14]  = k13
J[5,17]  = k20*y[6]

J[6,6]   = -k6*y[7]-k8*y[9]-k14*y[1]-k20*y[17]
J[6,7]   = -k6*y[6]
J[6,9]   = -k8*y[6]
J[6,1]   = -k14*y[6]
J[6,17]  = -k20*y[6]
J[6,2]   = k3*y[5]
J[6,5]   = k3*y[2]
J[6,16]  = 2k18

J[7,7]   = -k4-k5-k6*y[6]
J[7,6]   = -k6*y[7]
J[7,14]  = k13

J[8,7]   = k4+k5+k6*y[6]
J[8,6]   = k6*y[7]
J[8,9]   = k7

J[9,9]   = -k7-k8*y[6]
J[9,6]   = -k8*y[9]

J[10,10] = -k12*y[2]
J[10,2]  = -k12*y[10]+k9*y[11]
J[10,9]  = k7
J[10,11] = k9*y[2]

J[11,11] = -k9*y[2]-k10*y[1]
J[11,2]  = -k9*y[11]
J[11,1]  = -k10*y[11]
J[11,9]  = k8*y[6]
J[11,6]  = k8*y[9]
J[11,13] = k11

J[12,11] = k9*y[2]
J[12,2]  = k9*y[11]

J[13,13] = -k11
J[13,11] = k10*y[1]
J[13,1]  = k10*y[11]

J[14,14] = -k13
J[14,10] = k12*y[2]
J[14,2]  = k12*y[10]
```

```
    J[15,1]   = k14*y[6]
    J[15,6]   = k14*y[1]

    J[16,16] = -k18-k19
    J[16,4]   = k16

    J[17,17] = -k20*y[6]
    J[17,6]   = -k20*y[17]

    J[18,17] = k20*y[6]
    J[18,6]   = k20*y[17]

    J[19,19] = -k21-k22-k24*y[1]
    J[19,1]   = -k24*y[19]+k23*y[4]
    J[19,4]   = k23*y[1]
    J[19,20] = k25

    J[20,20] = -k25
    J[20,1]   = k24*y[19]
    J[20,19] = k24*y[1]

    return
end

u0 = zeros(20)
u0[2]   = 0.2
u0[4]   = 0.04
u0[7]   = 0.1
u0[8]   = 0.3
u0[9]   = 0.01
u0[17] = 0.007
prob = ODEProblem(ODEFunction(f, jac=fjac),u0,(0.0,60.0))

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 fail.

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

```
Any[]
```

The EPIRK and exponential methods also fail:

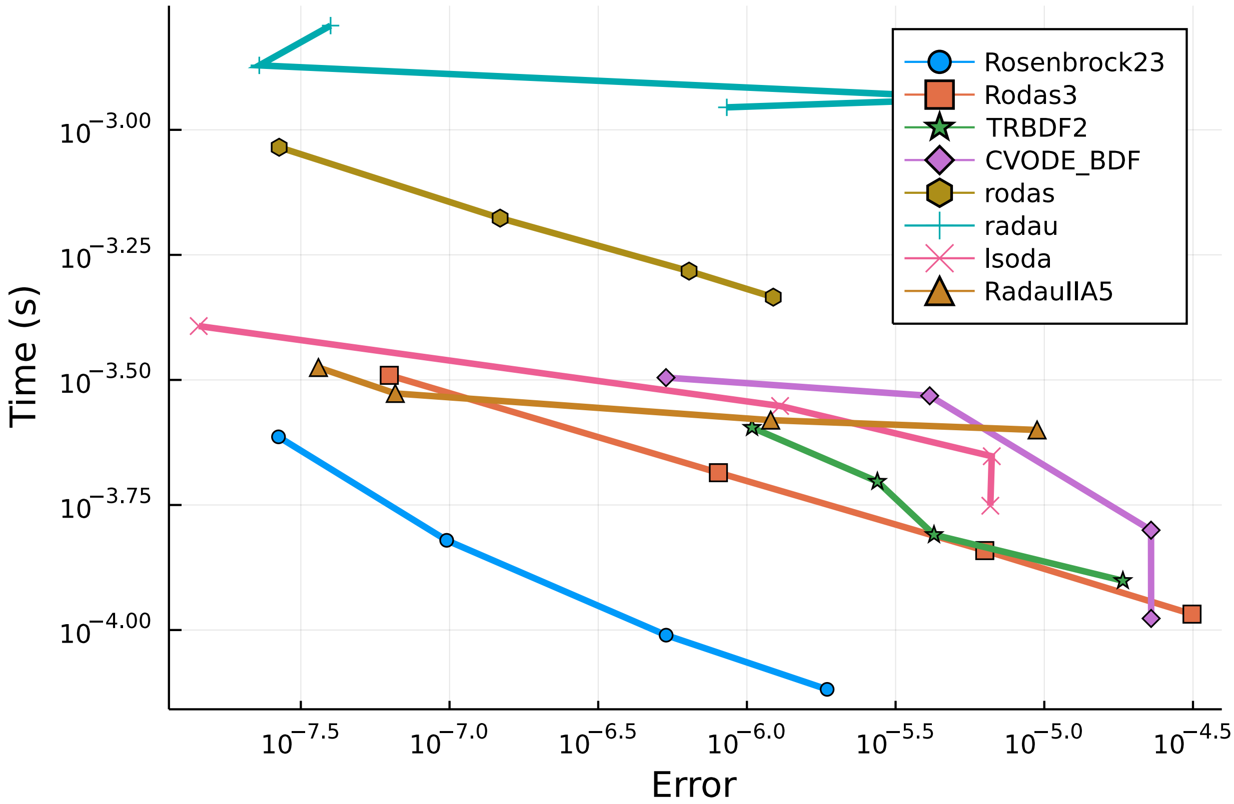
```
sol = solve(prob,EXPRB53s3(),dt=2.0^(-8));
sol = solve(prob,EPIRK4s3B(),dt=2.0^(-8));
sol = solve(prob,EPIRK5P2(),dt=2.0^(-8));
```

```
Error: InexactError: trunc(Int64, Inf)
```

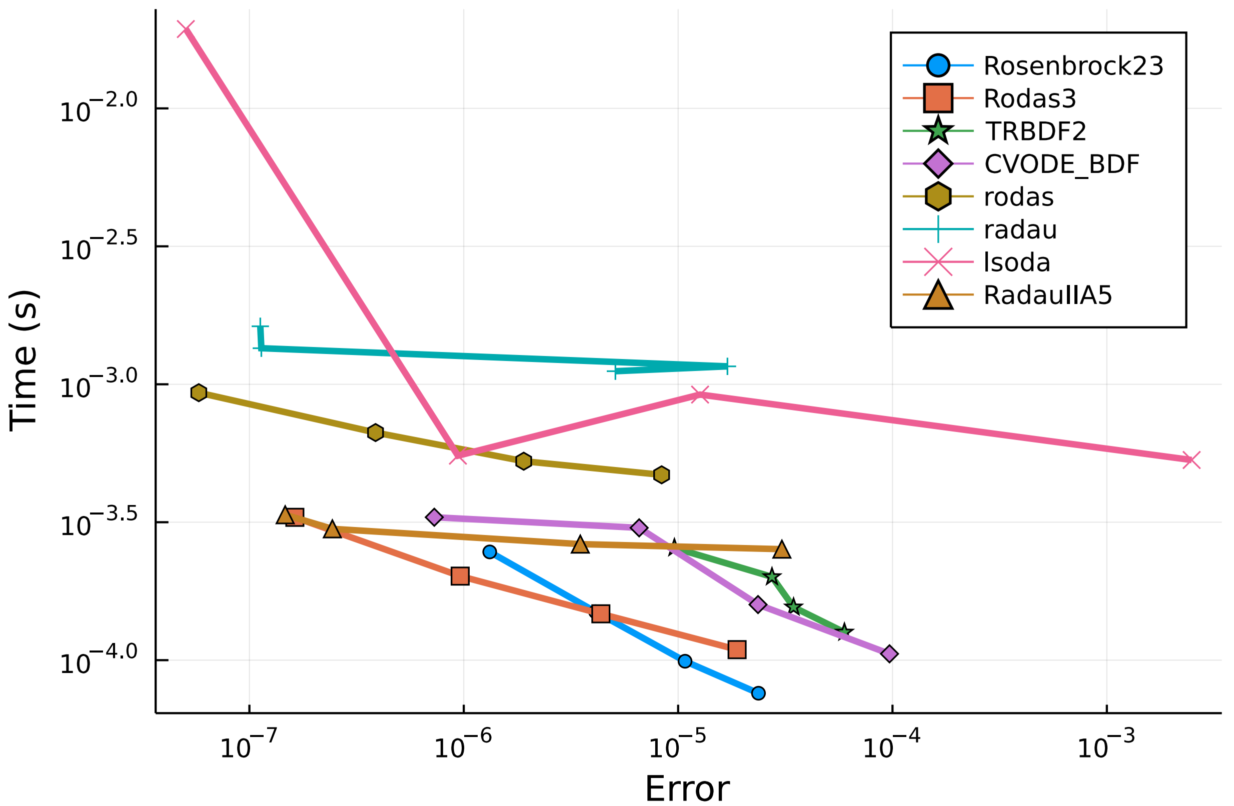
0.2 High Tolerances

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=>lsoda()),
          Dict(:alg=>RadauIIA5()),
          ]
wp = WorkPrecisionSet(prob,abstols,reltols,setups;verbose=false,
                      save_everystep=false,appxsol=test_sol,maxiters=Int(1e5),numruns=10)
plot(wp)
```

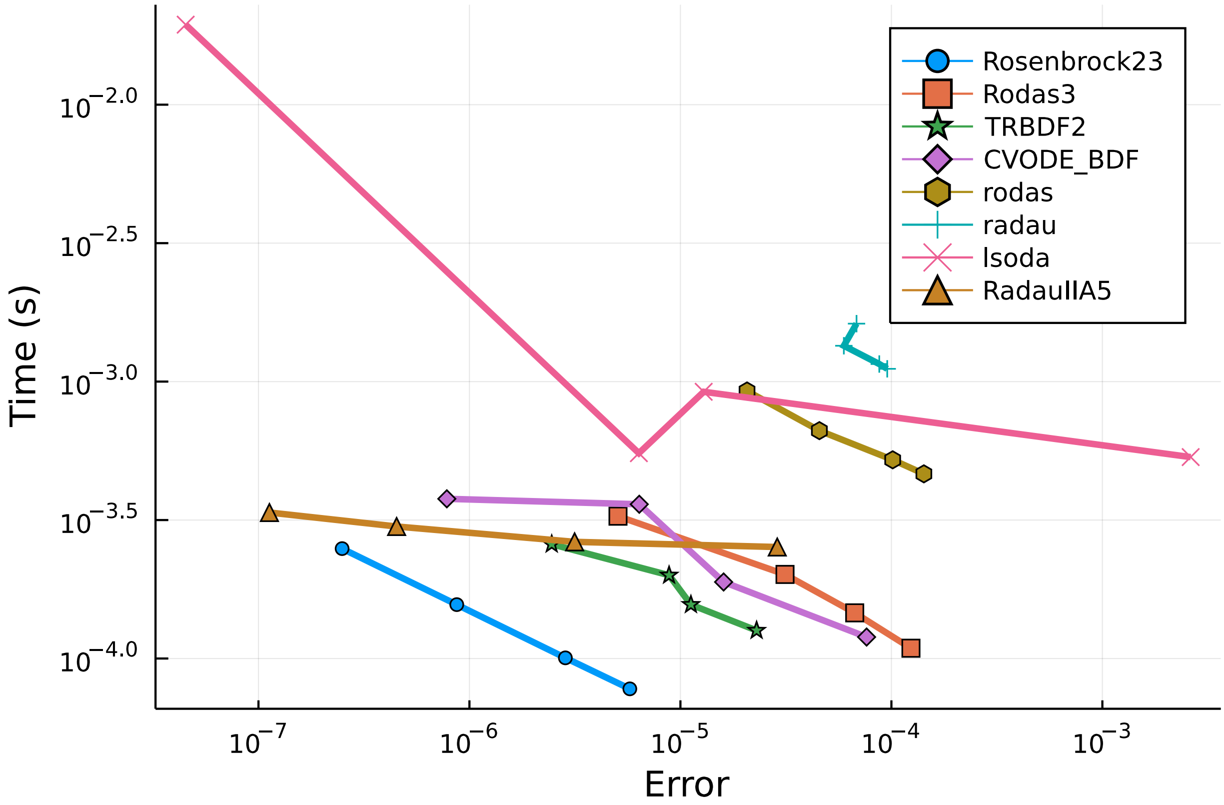



```
wp = WorkPrecisionSet(prob,abstols,reltols,setups;dense = false,verbose = false,
                      appxsol=test_sol,maxiters=Int(1e5),error_estimate=:l2,numruns=10)
plot(wp)
```

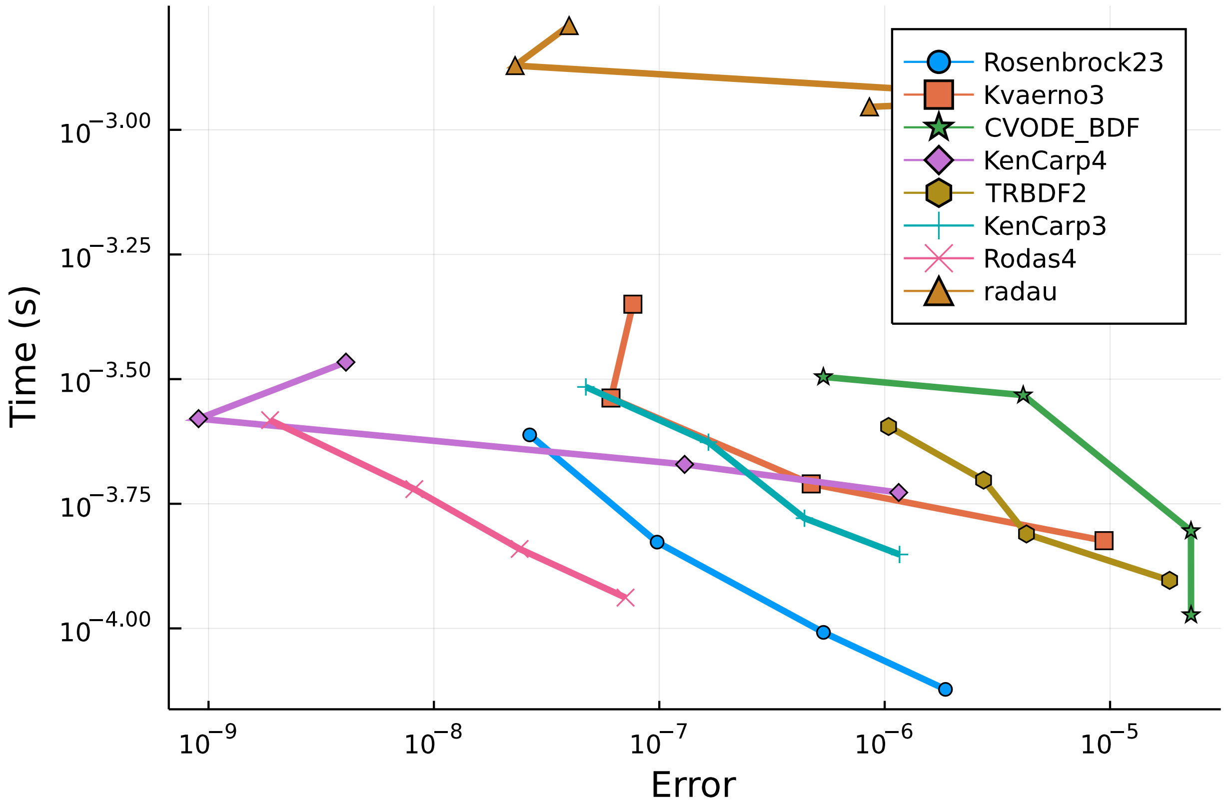



```
wp = WorkPrecisionSet(prob,abstols,reltols,setups;verbose=false,
                      appxsol=test_sol,maxiters=Int(1e5),error_estimate=:L2,numruns=10)
```

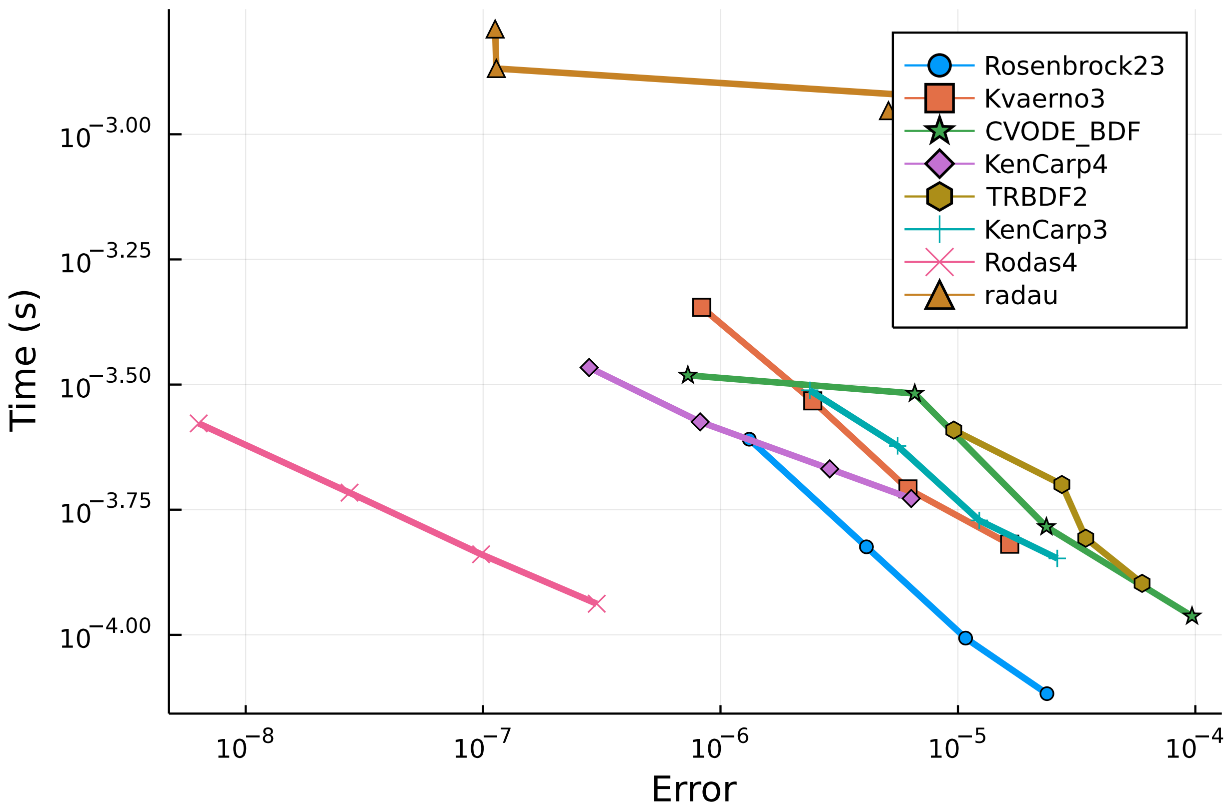
```
plot(wp)
```




```
setups = [Dict(:alg=>Rosenbrock23()),
          Dict(:alg=>Kvaerno3()),
          Dict(:alg=>CVODE_BDF()),
          Dict(:alg=>KenCarp4()),
          Dict(:alg=>TRBDF2()),
          Dict(:alg=>KenCarp3()),
          Dict(:alg=>Rodas4()),
          Dict(:alg=>radau())]
wp = WorkPrecisionSet(prob,abstols,reltols,setups;
                      save_everystep=false,appxsol=test_sol,maxiters=Int(1e5),numruns=10)
plot(wp)
```

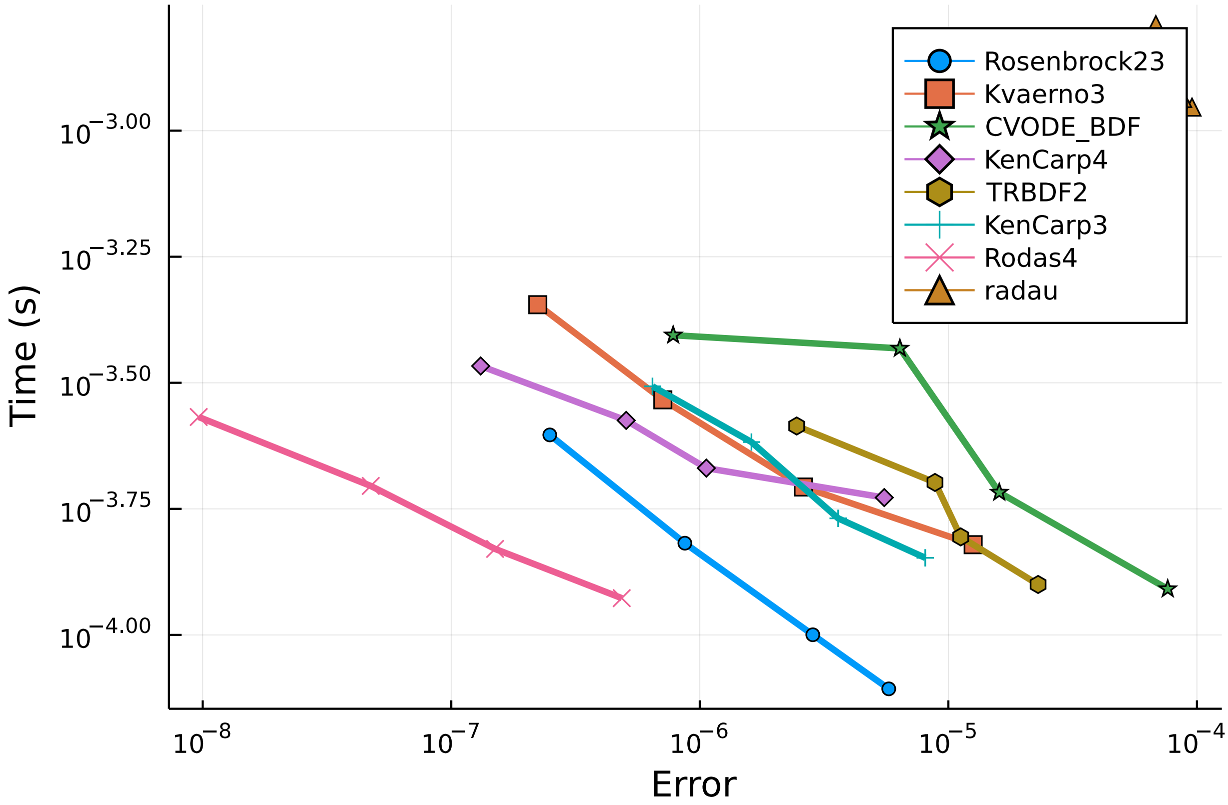



```
wp = WorkPrecisionSet(prob,abstols,reltols,setups;dense = false,verbose = false,
                      appxsol=test_sol,maxiters=Int(1e5),error_estimate=:l2,numruns=10)
plot(wp)
```



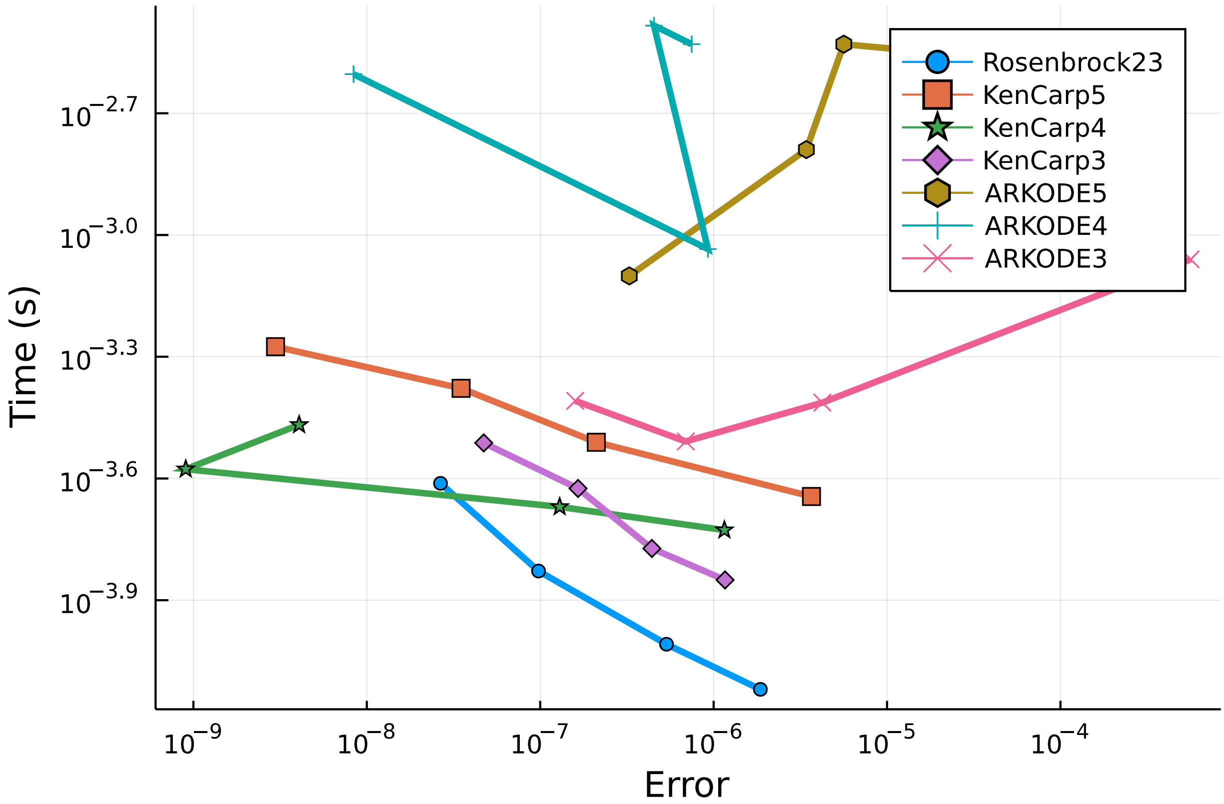

```
wp = WorkPrecisionSet(prob,abstols,reltols,setups;
                      appxsol=test_sol,maxiters=Int(1e5),error_estimate=:L2,numruns=10)
```

```julia
plot(wp)
```

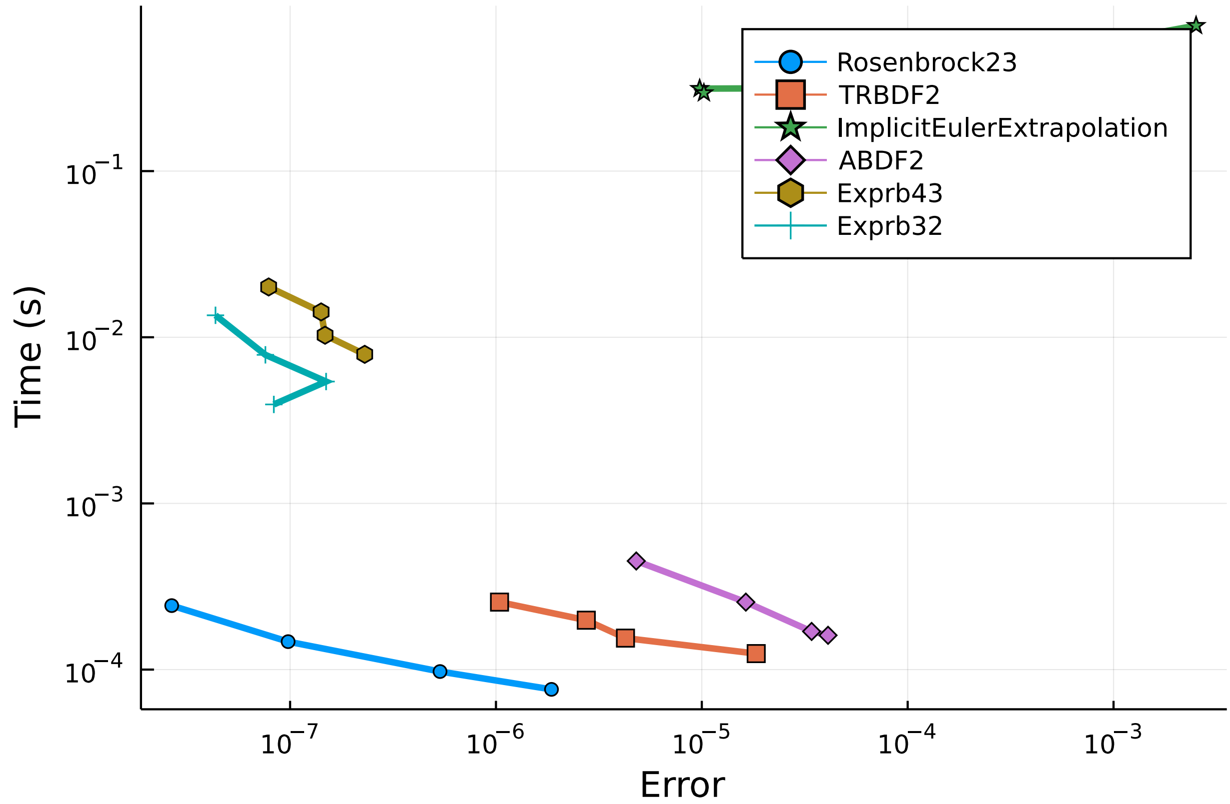



```julia
setups = [Dict(:alg=>Rosenbrock23()),
          Dict(:alg=>KenCarp5()),
          Dict(:alg=>KenCarp4()),
          Dict(:alg=>KenCarp3()),
          Dict(:alg=>ARKODE(order=5)),
          Dict(:alg=>ARKODE()),
          Dict(:alg=>ARKODE(order=3))]
names = ["Rosenbrock23" "KenCarp5" "KenCarp4" "KenCarp3" "ARKODE5" "ARKODE4" "ARKODE3"]
wp = WorkPrecisionSet(prob,abstols,reltols,setups;

names=names,save_everystep=false,appxsol=test_sol,maxiters=Int(1e5),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()),
          #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)
```

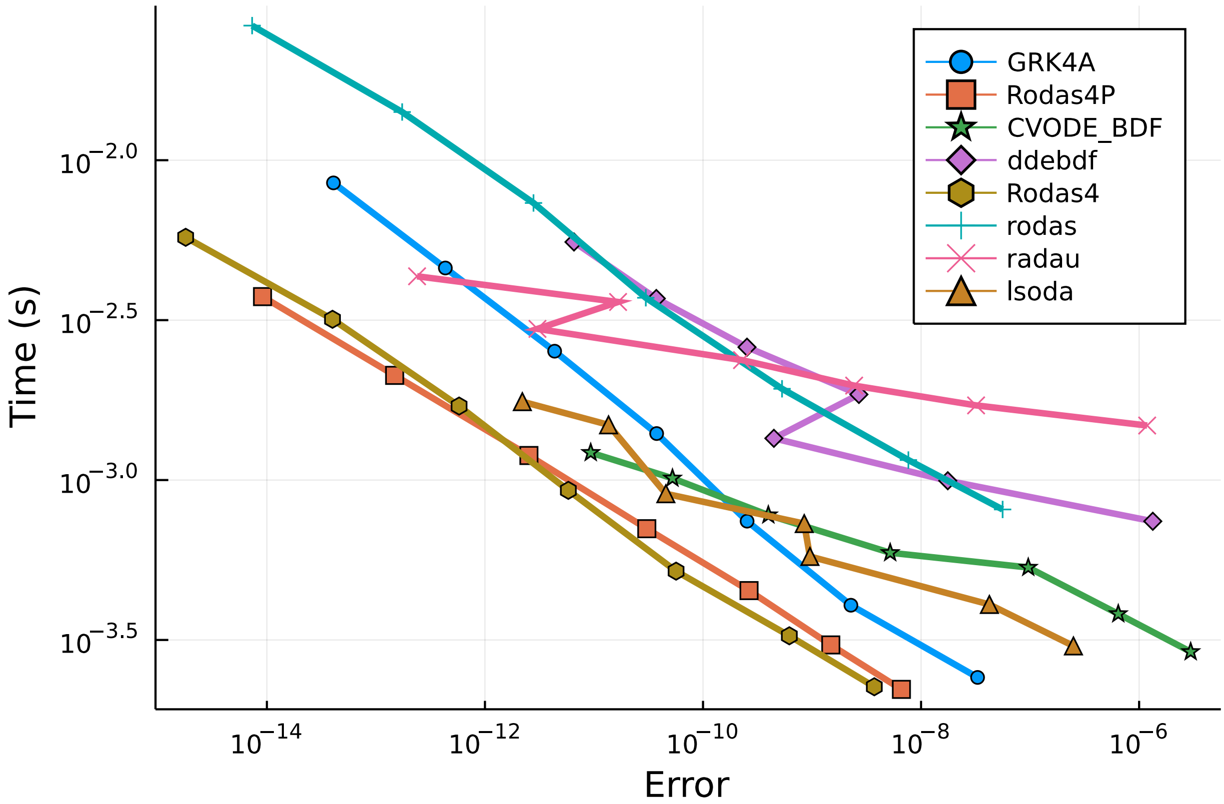


0.2.1 Low Tolerances

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

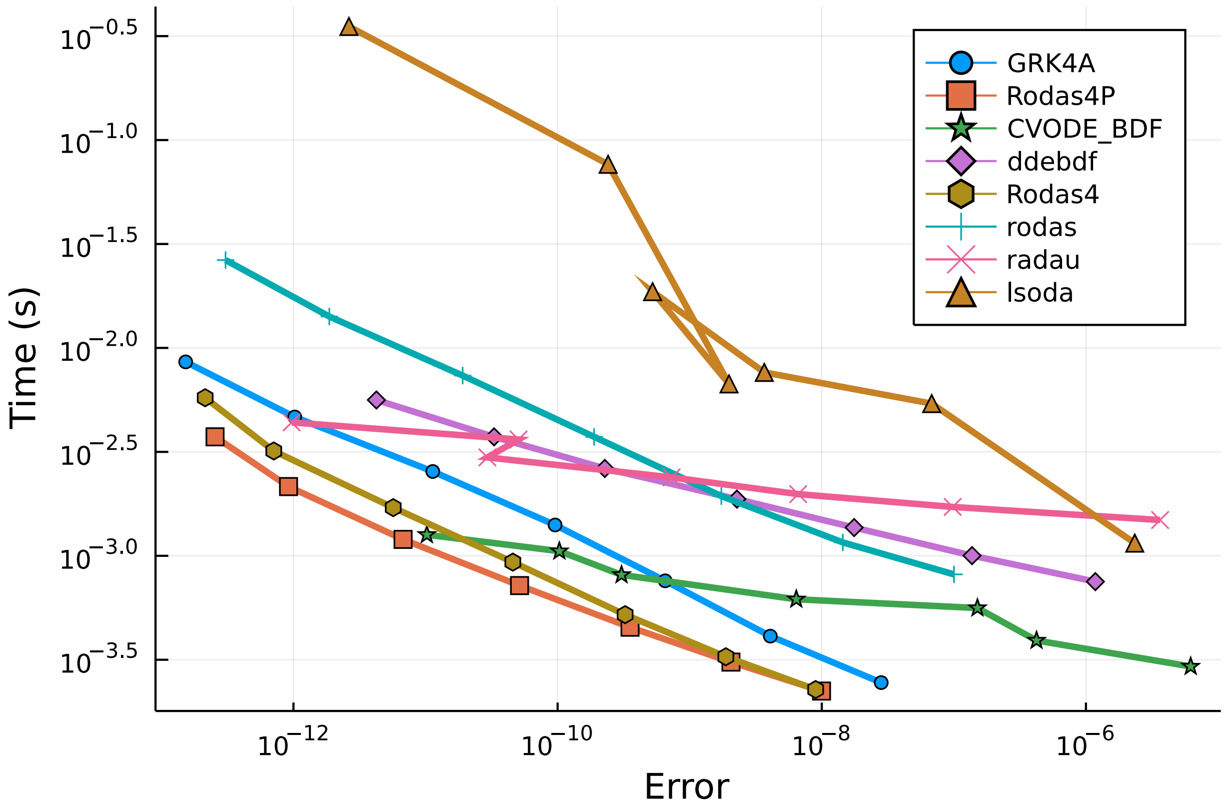
```
abstols = 1.0 ./ 10.0 .^ (7:13)
reltols = 1.0 ./ 10.0 .^ (4:10)

setups = [Dict(:alg=>GRK4A()),
          Dict(:alg=>Rodas4P()),
          Dict(:alg=>CVODE_BDF()),
          Dict(:alg=>ddebdf()),
          Dict(:alg=>Rodas4()),
          Dict(:alg=>rodas()),
          Dict(:alg=>radau()),
          Dict(:alg=>lsoda())
          ]
wp = WorkPrecisionSet(prob,abstols,reltols,setups;verbose=false,
                      save_everystep=false,appxsol=test_sol,maxiters=Int(1e5),numruns=10)
plot(wp)
```



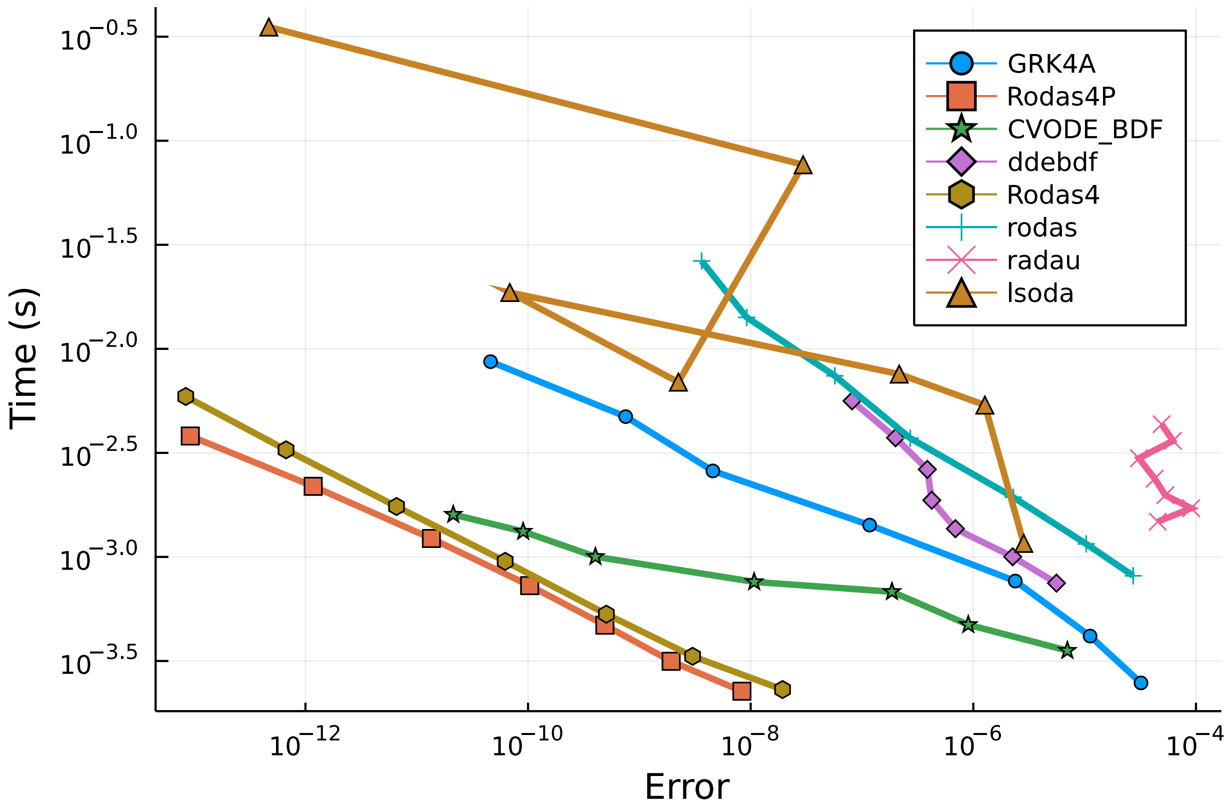

```
wp = WorkPrecisionSet(prob,abstols,reltols,setups;verbose=false,

dense=false,appxsol=test_sol,maxiters=Int(1e5),error_estimate=:l2,numruns=10)
plot(wp)
```

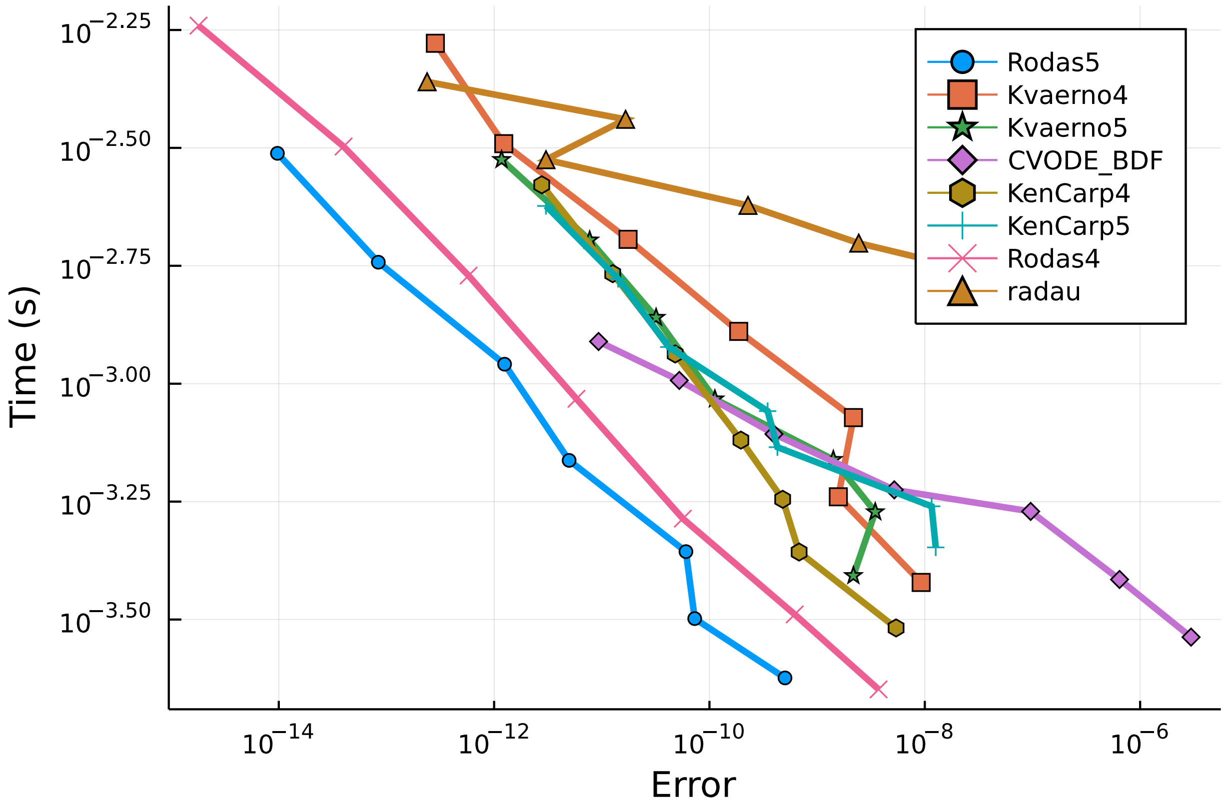



```
wp = WorkPrecisionSet(prob,abstols,reltols,setups;verbose=false,
```

```
                              appxsol=test_sol,maxiters=Int(1e5),error_estimate=:L2,numruns=10)
plot(wp)
```

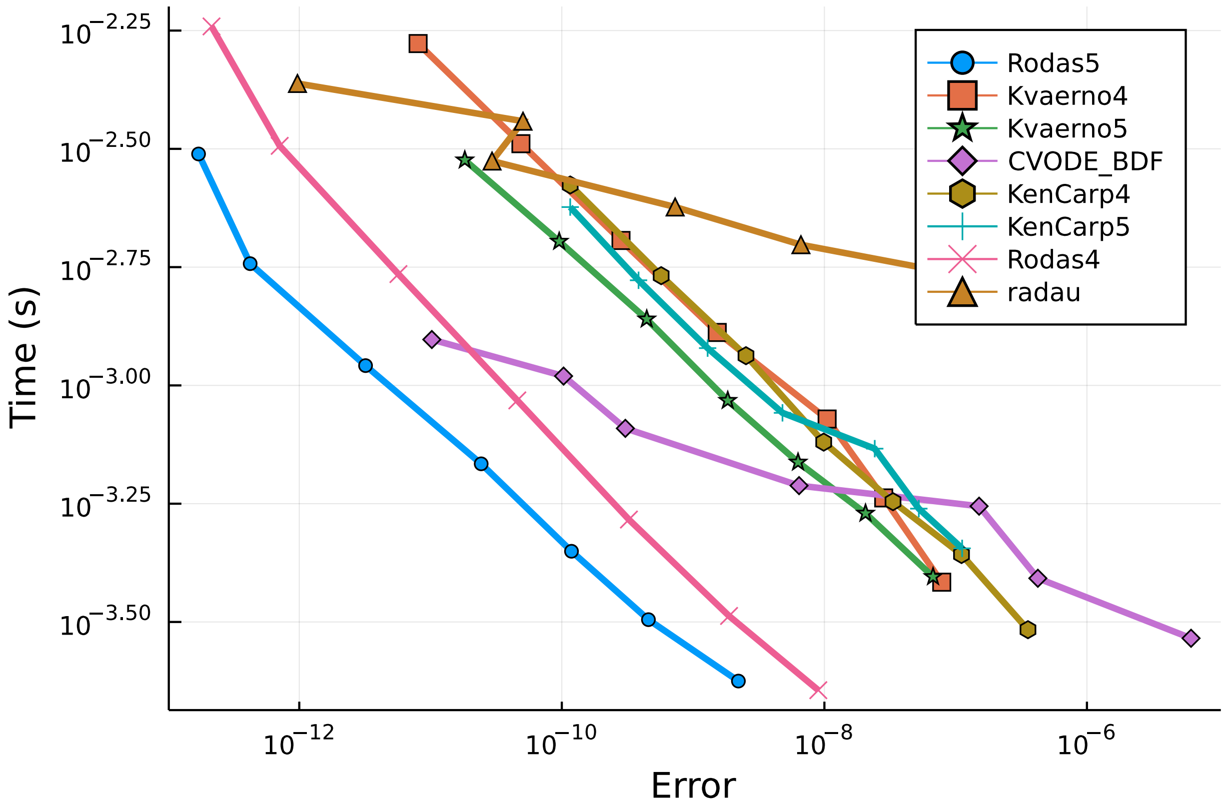



```
setups = [
          Dict(:alg=>Rodas5()),
          Dict(:alg=>Kvaerno4()),
          Dict(:alg=>Kvaerno5()),
          Dict(:alg=>CVODE_BDF()),
          Dict(:alg=>KenCarp4()),
          Dict(:alg=>KenCarp5()),
          Dict(:alg=>Rodas4()),
          Dict(:alg=>radau())]
wp = WorkPrecisionSet(prob,abstols,reltols,setups;
                              save_everystep=false,appxsol=test_sol,maxiters=Int(1e5),numruns=10)
plot(wp)
```



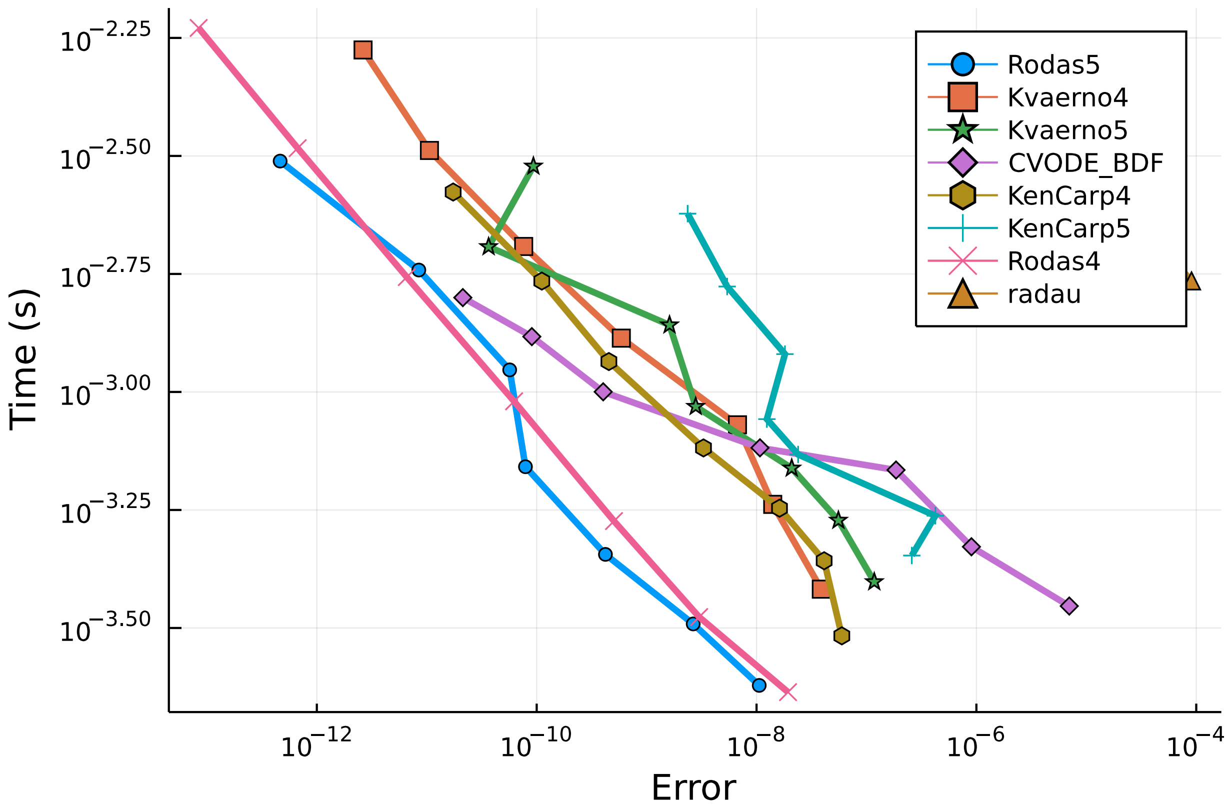

```
wp = WorkPrecisionSet(prob,abstols,reltols,setups;verbose=false,

dense=false,appxsol=test_sol,maxiters=Int(1e5),error_estimate=:l2,numruns=10)
plot(wp)
```




```
wp = WorkPrecisionSet(prob,abstols,reltols,setups;
```

```
                         appxsol=test_sol,maxiters=Int(1e5),error_estimate=:L2,numruns=10)
plot(wp)
```



The following algorithms were removed since they failed.

```
#setups = [#Dict(:alg=>Hairer4()),
          #Dict(:alg=>Hairer42()),
          #Dict(:alg=>Rodas3()),
          #Dict(:alg=>Cash4())
#]
#wp = WorkPrecisionSet(prob,abstols,reltols,setups;
#
save_everystep=false,appxsol=test_sol,maxiters=Int(1e5),numruns=10)
#plot(wp)
```

0.2.2 Conclusion

Sundials `CVODE_BDF` the best here. `lsoda` does well at high tolerances but then grows fast when tolerances get too low. `KenCarp4` or `Rodas5` is a decent substitute when necessary.

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","Pollution.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
  [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
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