POLLU Work-Precision Diagrams

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```
using OrdinaryDiffEq, DiffEqDevTools, Sundials, ParameterizedFunctions, Plots, ODE,
ODEInterfaceDiffEq, LSODA
gr() # gr(fmt=:png)
using LinearAlgebra
LinearAlgebra.BLAS.set_num_threads(1)
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]
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
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
```

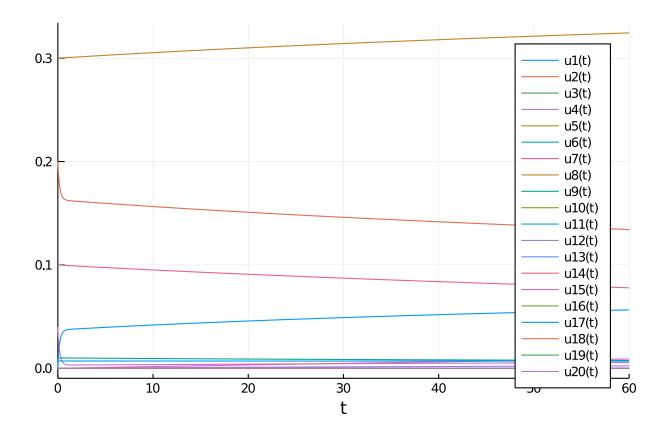
```
J[3,4] = k17
J[3,16] = k19
J[3,19] = k22
J[3,3] = -k15
J[4,4] = -k2*y[2]-k16-k17-k23*y[1]
J[4,2] = -k2*y[4]
J[4,1] = -k23*y[4]
J[4,3]
       = k15
J[5,5]
       = -k3*y[2]
J[5,2] = -k3*y[5]
J[5,7] = 2k4+k6*y[6]
J[5,6] = k6*y[7]+k20*y[17]
J[5,9] = k7
J[5,14] = k13
J[5,17] = k20*y[6]
J[6,6] = -k6*y[7]-k8*y[9]-k14*y[1]-k20*y[17]
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]

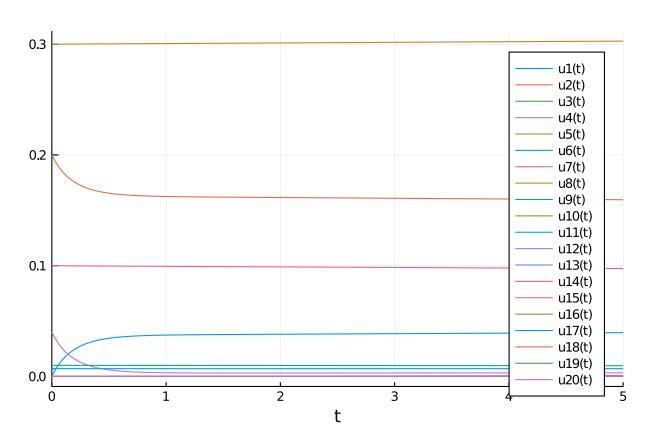
J[11,6] = k8*y[9]
J[11,13] = k11
J[12,11] = k9*y[2]
J[12,2] = k9*y[11]
J[13,13] = -k11
J[13,11] = k10*y[1]
J[13,1] = k10*y[11]
J[14,14] = -k13
J[14,10] = k12*y[2]
```

```
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);
8-element Array{Float64,1}:
0.1
 0.01
 0.001
 0.0001
 1.0e-5
 1.0e-6
 1.0e-7
 1.0e-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(:alq=>ROCK2()),
#Dict(:alg=>ROCK4())
#Dict(:alq=>ESERK5())
O-element Array{Any,1}
The EPIRK and exponential methods also fail:
sol = solve(prob, EXPRB53s3(), dt=2.0^(-8));
Error: InexactError: trunc(Int64, Inf)
sol = solve(prob, EPIRK4s3B(), dt=2.0^(-8));
Error: InexactError: trunc(Int64, Inf)
sol = solve(prob, EPIRK5P2(), dt=2.0^(-8));
retcode: Success
Interpolation: 3rd order Hermite
t: 15361-element Array{Float64,1}:
  0.0
  0.00390625
  0.0078125
  0.01171875
  0.015625
  0.01953125
  0.0234375
  0.02734375
  0.03125
  0.03515625
 59.96875
 59.97265625
 59.9765625
 59.98046875
 59.984375
 59.98828125
 59.9921875
 59.99609375
```

```
60.0
```

u: 15361-element Array{Array{Float64,1},1}: [0.0, 0.2, 0.0, 0.04, 0.0, 0.0, 0.1, 0.3, 0.01, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.007, 0.0, 0.0, 0.0] [0.0008219805131540299, 0.19917801095752233, 2.0563502567328148e-10, 0.039]17956419724961, 2.3582619681121442e-7, 2.9410765063389164e-7, 0.09999845709 043506612553868e-8, 1.216654286569352e-7, 1.9129510494780006e-10, 1.0123808 201200793e-7, 5.350876495558082e-9, 3.087407735661497e-17, 0.00699999486790 5456, 5.132094544073881e-9, 2.978581368352407e-9, 4.285419171616549e-12] [0.0016247338242586589, 0.19837521677879572, 2.612072012079205e-10, 0.0383]8030124412858, 3.4971496424010073e-7, 4.6379695201199464e-7, 0.099995526354 58558, 0.30000448587467143, 0.009999483726072282, 4.4657968858173745e-8, 3. 314357123409278e-8, 4.715760800673718e-7, 1.3982133045801176e-9, 4.35000980 3873253e-7, 3.637387900607056e-8, 3.02479855802291e-17, 0.00699998169495262 8, 1.8305047372094373e-8, 1.1493115150672013e-8, 6.586916883204175e-11] $[0.002407958732495669,\ 0.1975919095090435,\ 3.154375436634084e-10,\ 0.037601]$ 54313554651, 4.063896496720431e-7, 5.450652668055192e-7, 0.0999918876051537 5, 0.3000081345333246, 0.009999000674914008, 5.423073753127883e-8, 3.953344 234000373e-8, 9.405378956905758e-7, 4.019941772178222e-9, 8.946362921399464 e-7, 1.022230169770184e-7, 2.963424332875256e-17, 0.00699996440700378, 3.55 929962200743e-8, 2.4876007075065313e-8, 3.197475864984921e-10] [0.003171744493887124, 0.1968280004910967, 3.683293249789368e-10, 0.036842]64477850668, 4.3074308952271334e-7, 5.770142622377038e-7, 0.099987935557457 69, 0.30001210009903406, 0.009998466922328109, 5.826989959035465e-8, 4.2154 008016303866e-8, 1.4625566429623716e-6, 8.055731505071132e-9, 1.40925283037 3719e-6, 2.0259372371519383e-7, 2.903611344736133e-17, 0.006999945284289526 , 5.471571047264492e-8, 4.243113301483705e-8, 9.6721405195278e-10] $\hbox{\tt [0.003916411612522152, 0.19608317317188564, 4.199027567232139e-10, 0.03610] }$ 2984774372494, 4.377436299333023e-7, 5.828832755232177e-7, 0.09998388521210 591, 0.30001616781761936, 0.009997916829455644, 5.933835798375604e-8, 4.276 4607301600245e-8, 2.0016541543959203e-6, 1.3363286615438824e-8, 1.940063063 1287573e-6, 3.338844922954957e-7, 2.845321984913385e-17, 0.0069999255695067 56, 7.443049324392098e-8, 6.345530181035366e-8, 2.2562558299901686e-9] $[0.004642405059285701,\ 0.19535698700687829,\ 4.701872267485031 \text{e}-10,\ 0.03538]$ 196494207218, 4.3599615353021897e-7, 5.758783078537109e-7, 0.09997984694079 727, 0.30002022735435296, 0.009997368049509693, 5.8909962388343646e-8, 4.23 7152084922936e-8, 2.5393376067316203e-6, 1.977593916416651e-8, 2.4670633411 69356e-6, 4.919744863822924e-7, 2.788494570784191e-17, 0.006999905901180717 , 9.409881928300559e-8, 8.725661950672292e-8, 4.463395577854287e-9] $[0.005350228551009552,\ 0.1946489421275031,\ 5.192165244761254e-10,\ 0.034679]$ 01012916707, 4.3022917680639446e-7, 5.631689167361495e-7, 0.099975872878565 67, 0.3000242265067192, 0.00999682893422216, 5.779485557447839e-8, 4.152477 10322123e-8, 3.066852273486213e-6, 2.7146658586645518e-8, 2.98075628242511e $-6,\ 6.732501359597954e-7,\ 2.733092948771845e-17,\ 0.006999886581464048,\ 1.13$ 41853595155117e-7, 1.1316977012076304e-7, 7.877461431787497e-9] [0.006040406864840676, 0.1939585168088369, 5.670261038607765e-10, 0.033993]56729906623, 4.2291899338282446e-7, 5.484585573765662e-7, 0.099971984234016 64, 0.3000281439517046, 0.009996302894574066, 5.641740775276457e-8, 4.05106 59700017454e-8, 3.5806181839668297e-6, 3.535812741357323e-8, 3.477251964668 5567e-6, 8.748287134377105e-7, 2.6790726790238164e-17, 0.006999867733817418 , 1.322661825816341e-7, 1.405683346708844e-7, 1.278557353504999e-8] $\hbox{\tt [0.006713465378819361, 0.19328518802723454, 6.136515989812096e-10, 0.03332] }$ 510439182137, 4.152909854262616e-7, 5.335478076046044e-7, 0.099968186650105 64, 0.30003197391503733, 0.009995790853860426, 5.498765243303229e-8, 3.9469 76537302462e-8, 4.079662077209273e-6, 4.431972526378151e-8, 3.9554984252451 48e-6, 1.0944769689609055e-6, 2.626389554944705e-17, 0.006999849391717465, 1.5060828253459265e-7, 1.6887427672026182e-7, 1.9461487666521883e-8]

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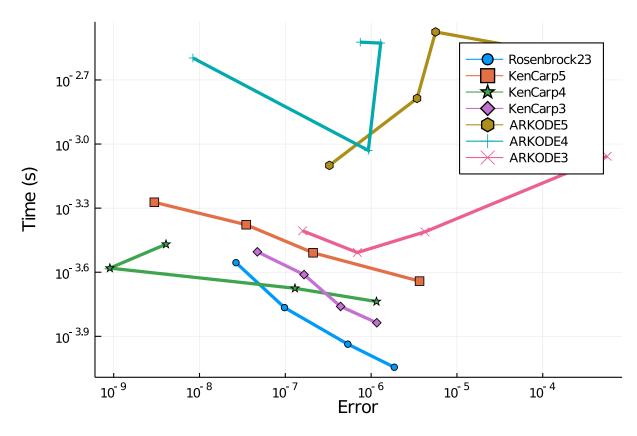
```
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0.00010074114286132725, 1.771572137484069e-6, 5.680446793668939e-5]
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, 0.00010074603809481543, 1.7716439320601548e-6, 5.680758831940337e-5]
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[0.05646255432713235,\ 0.13424841374736396,\ 4.139734296272654e-9,\ 0.0055231]
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8638511982452e-8, 0.0022305059184782802, 0.0002087162866581338, 1.396921045
7025133e-5, 0.008964884630137337, 4.352848183498503e-18, 0.0068992196990593
67, 0.00010078030094348328, 1.772146472774919e-6, 5.6829431118266636e-5]
```

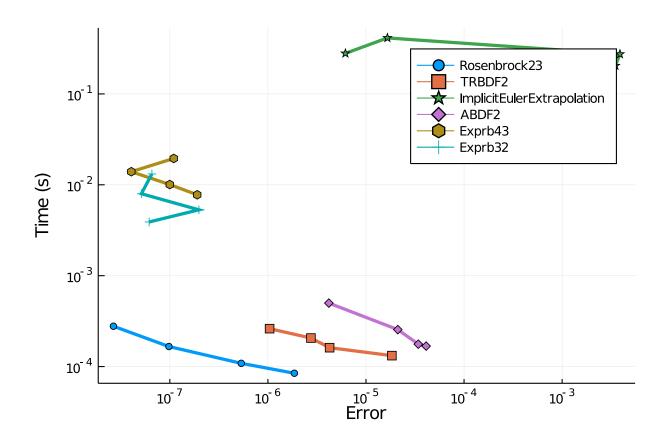
0.2 High Tolerances

```
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)
Error: Cannot find method(s) for rodas! I've tried to loadODESolvers(), but
 it didn't work. Please check ODEInterface.help_solversupport() and call lo
adODESolvers and check also this output. For further information see also 0
DEInterface.help_install.
plot(wp)
Error: UndefVarError: wp not defined
wp = WorkPrecisionSet(prob, abstols, reltols, setups; dense = false, verbose = false,
                      appxsol=test_sol,maxiters=Int(1e5),error_estimate=:12,numruns=10)
Error: Cannot find method(s) for rodas! I've tried to loadODESolvers(), but
 it didn't work. Please check ODEInterface.help_solversupport() and call lo
adODESolvers and check also this output. For further information see also O
DEInterface.help_install.
plot(wp)
Error: UndefVarError: wp not defined
wp = WorkPrecisionSet(prob,abstols,reltols,setups;verbose=false,
                      appxsol=test_sol,maxiters=Int(1e5),error_estimate=:L2,numruns=10)
Error: Cannot find method(s) for rodas! I've tried to loadODESolvers(), but
 it didn't work. Please check ODEInterface.help solversupport() and call lo
adODESolvers and check also this output. For further information see also 0
DEInterface.help_install.
plot(wp)
Error: UndefVarError: wp not defined
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)
```

```
adODESolvers and check also this output. For further information see also 0
DEInterface.help_install.
plot(wp)
Error: UndefVarError: wp not defined
wp = WorkPrecisionSet(prob, abstols, reltols, setups; dense = false, verbose = false,
                      appxsol=test_sol,maxiters=Int(1e5),error_estimate=:12,numruns=10)
Error: Cannot find method(s) for radau! I've tried to loadODESolvers(), but
 it didn't work. Please check ODEInterface.help_solversupport() and call lo
adODESolvers and check also this output. For further information see also {\tt O}
DEInterface.help_install.
plot(wp)
Error: UndefVarError: wp not defined
wp = WorkPrecisionSet(prob,abstols,reltols,setups;
                      appxsol=test_sol,maxiters=Int(1e5),error_estimate=:L2,numruns=10)
Error: Cannot find method(s) for radau! I've tried to loadODESolvers(), but
 it didn't work. Please check ODEInterface.help_solversupport() and call lo
adODESolvers and check also this output. For further information see also 0
DEInterface.help_install.
plot(wp)
Error: UndefVarError: wp not defined
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)
```

Error: Cannot find method(s) for radau! I've tried to loadODESolvers(), but it didn't work. Please check ODEInterface.help_solversupport() and call lo



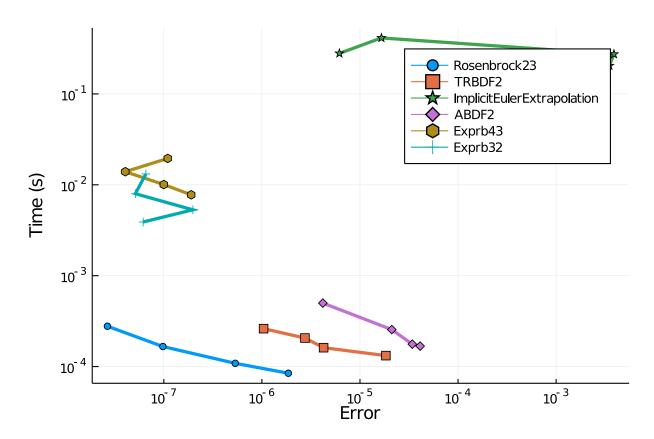


0.2.1 Low Tolerances

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

Error: Cannot find method(s) for ddebdf! I've tried to loadODESolvers(), bu t it didn't work. Please check ODEInterface.help_solversupport() and call 1 oadODESolvers and check also this output. For further information see also ODEInterface.help_install.

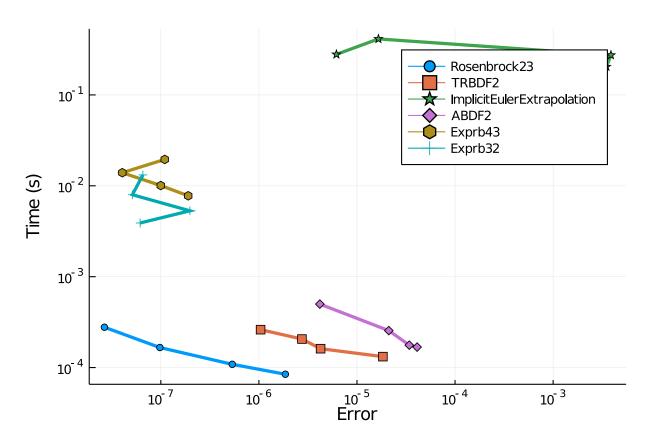
```
plot(wp)
```



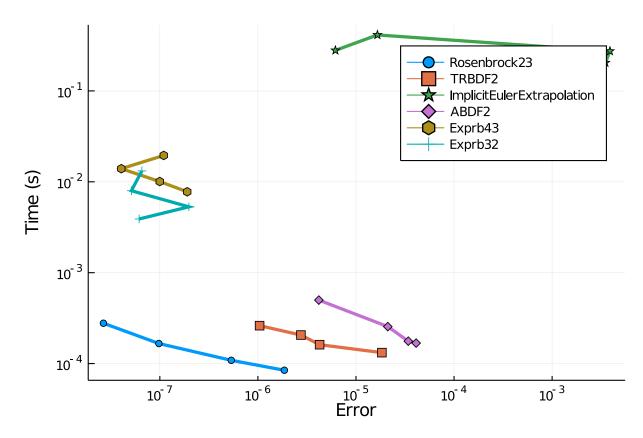
wp = WorkPrecisionSet(prob,abstols,reltols,setups;verbose=false,

dense=false,appxsol=test_sol,maxiters=Int(1e5),error_estimate=:12,numruns=10)

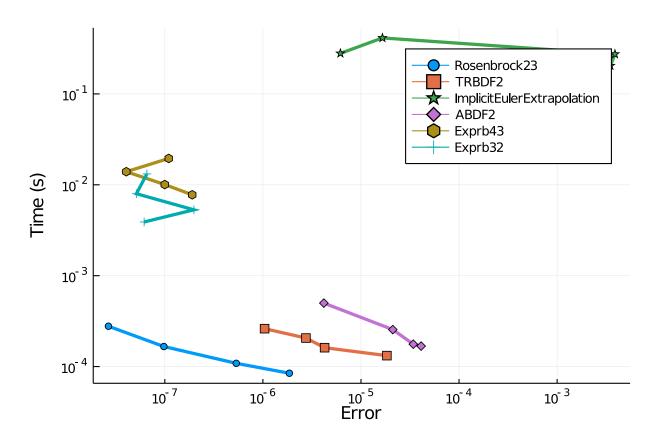
Error: Cannot find method(s) for ddebdf! I've tried to loadODESolvers(), bu t it didn't work. Please check ODEInterface.help_solversupport() and call l oadODESolvers and check also this output. For further information see also ODEInterface.help_install.



Error: Cannot find method(s) for ddebdf! I've tried to loadODESolvers(), bu t it didn't work. Please check ODEInterface.help_solversupport() and call l oadODESolvers and check also this output. For further information see also ODEInterface.help_install.



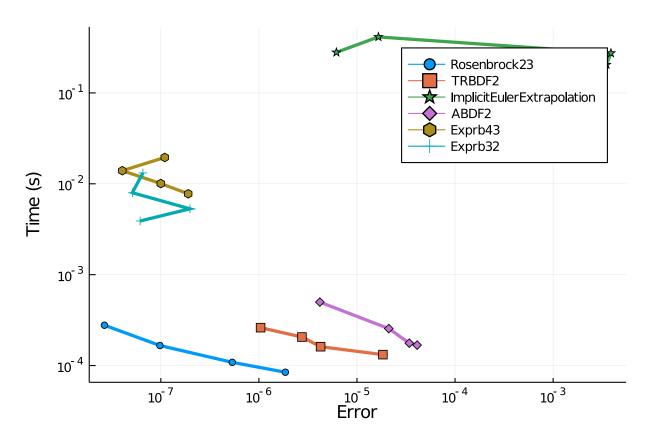
Error: Cannot find method(s) for radau! I've tried to loadODESolvers(), but it didn't work. Please check ODEInterface.help_solversupport() and call lo adODESolvers and check also this output. For further information see also O DEInterface.help_install.



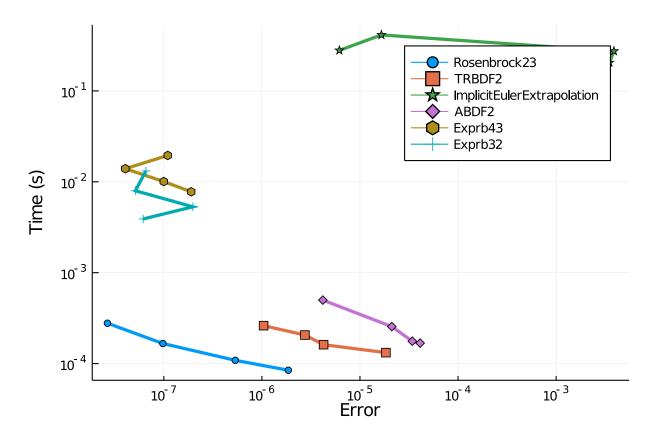
wp = WorkPrecisionSet(prob,abstols,reltols,setups;verbose=false,

dense=false,appxsol=test_sol,maxiters=Int(1e5),error_estimate=:12,numruns=10)

Error: Cannot find method(s) for radau! I've tried to loadODESolvers(), but it didn't work. Please check ODEInterface.help_solversupport() and call lo adODESolvers and check also this output. For further information see also O DEInterface.help_install.



Error: Cannot find method(s) for radau! I've tried to loadODESolvers(), but it didn't work. Please check ODEInterface.help_solversupport() and call lo adODESolvers and check also this output. For further information see also O DEInterface.help_install.



The following algorithms were removed since they failed.

0.2.2 Conclusion

Sundials CVODE_BDF the best here. 1soda does well at high tolerances but then grows fast when tolerances get too low. KenCarp4 or Rodas5 is a decent substitute when necessary.

```
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/JuliaDenchmarks.jl repository,

```
using DiffEqBenchmarks
DiffEqBenchmarks.weave_file("StiffODE","Pollution.jmd")
```

Computer Information:

```
Julia Version 1.4.2
Commit 44fa15b150* (2020-05-23 18:35 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-8.0.1 (ORCJIT, skylake)
Environment:
    JULIA_DEPOT_PATH = /builds/JuliaGPU/DiffEqBenchmarks.jl/.julia
    JULIA_CUDA_MEMORY_LIMIT = 2147483648
    JULIA_PROJECT = @.
    JULIA_NUM_THREADS = 4
```

Package Information:

```
Status: `/builds/JuliaGPU/DiffEqBenchmarks.jl/benchmarks/StiffODE/Project.toml`
[eb300fae-53e8-50a0-950c-e21f52c2b7e0] DiffEqBiological 4.3.0
[f3b72e0c-5b89-59e1-b016-84e28bfd966d] DiffEqDevTools 2.22.0
[5a33fad7-5ce4-5983-9f5d-5f26ceab5c96] GeometricIntegratorsDiffEq 0.1.0
[7f56f5a3-f504-529b-bc02-0b1fe5e64312] LSODA 0.6.1
[c030b06c-0b6d-57c2-b091-7029874bd033] ODE 2.5.0
[09606e27-ecf5-54fc-bb29-004bd9f985bf] ODEInterfaceDiffEq 3.7.0
[1dea7af3-3e70-54e6-95c3-0bf5283fa5ed] OrdinaryDiffEq 5.41.0
[65888b18-ceab-5e60-b2b9-181511a3b968] ParameterizedFunctions 5.3.0
[91a5bcdd-55d7-5caf-9e0b-520d859cae80] Plots 1.5.3
[b4db0fb7-de2a-5028-82bf-5021f5cfa881] ReactionNetworkImporters 0.1.5
[c3572dad-4567-51f8-b174-8c6c989267f4] Sundials 4.2.5
[a759f4b9-e2f1-59dc-863e-4aeb61b1ea8f] TimerOutputs 0.5.6
[37e2e46d-f89d-539d-b4ee-838fcccc9c8e] LinearAlgebra
```