VanDerPol Work-Precision Diagrams

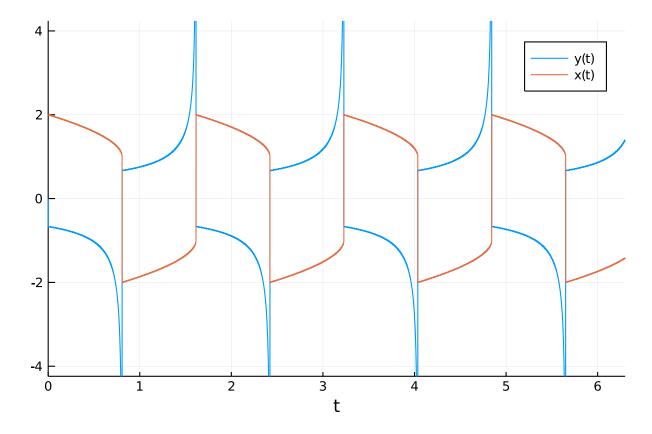
Chris Rackauckas

July 4, 2020

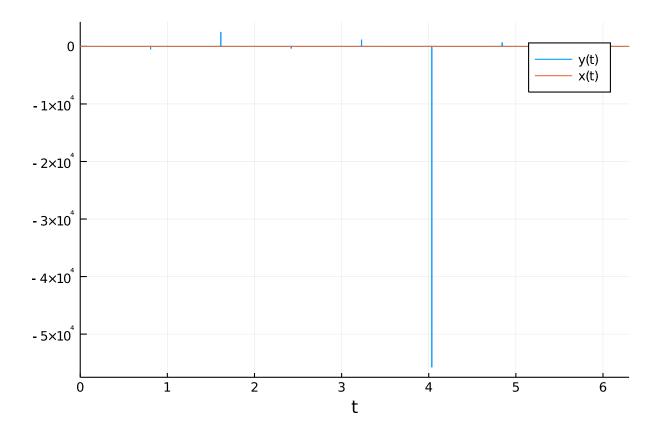
```
using OrdinaryDiffEq, DiffEqDevTools, Sundials, ParameterizedFunctions, Plots, ODE,
ODEInterfaceDiffEq, ODEInterface, LSODA
Error: ArgumentError: Package ODEInterface not found in current path:
- Run `import Pkg; Pkg.add("ODEInterface")` to install the ODEInterface pac
kage.
gr()
using LinearAlgebra
LinearAlgebra.BLAS.set_num_threads(1)
van = @ode_def begin
 dy = \mu * ((1-x^2)*y - x)
 dx = 1*y
end \mu
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);
```

```
retcode: Success
Interpolation: 3rd order Hermite
t: 67-element Array{Float64,1}:
0.0
5.749667114830345e-12
4.791703937695112e-10
6.937321127653181e-9
3.441348932456689e-8
1.242075614319914e-7
2.7833002915369977e-7
5.271605941797656e-7
7.759911592058314e-7
1.1947346368487868e-6
```

```
0.0019907624998313864
 0.002078339702740356
 0.002339121422761175
 0.0029039110661651796
 0.0038578803826986837
0.004811849699232188
 0.006545323108711468
 0.008114583820483115
 0.008115757710091452
u: 67-element Array{Array{Float64,1},1}:
 [0.0, 2.0]
 [-1.1499235054215125e-5, 2.0]
 [-0.0009576523046803073, 1.9999999999997706]
 [-0.01373125939606262, 1.999999999952206]
 [-0.0653932867684174, 1.9999999988554367]
 [-0.20738269006768967, 1.9999999863225233]
 [-0.3774085043828771, 1.9999999402494826]
 [-0.5295224816821857, 1.9999998250670898]
 [-0.6016433974890778, 1.9999996832203253]
 [-0.6480986302315671, 1.999999419542989]
 [-0.6674068309061841, 1.9986723129231863]
 [-0.6674331992515048, 1.998613862027106]
 [-0.6674990719448132, 1.9984397938438712]
 [-0.667628994834417, 1.9980627178538726]
 [-0.6680671424810317, 1.997425540358304]
 [-0.6686940561037535, 1.9967880235133677]
 [-0.6703810243516862, 1.9956287106603585]
 [-0.5871133352574344, 1.994578210009938]
 [-0.5871133352574344, 1.994578210009938]
sol = solve(prob, ARKODE(nonlinear_convergence_coefficient =
1e-6),abstol=1e-4,reltol=1e-1);
retcode: Success
Interpolation: 3rd order Hermite
t: 4205-element Array{Float64,1}:
0.0
5.749667114830345e-12
 4.791703937695112e-10
 6.950174703123355e-9
 3.7680390665050866e-8
 1.6391466409237974e-7
 4.069899042614494e-7
 8.711024624587683e-7
 1.5770981486067485e-6
 2.7874280262519495e-6
 6.277376975965755
 6.28032019042069
 6.283183377375016
 6.286046564329342
 6.288830917074367
 6.291615269819391
 6.293711452364543
 6.295807634909695
 6.3
```

```
u: 4205-element Array{Array{Float64,1},1}:
 [0.0, 2.0]
 [-1.1499235054215125e-5, 2.0]
 [-0.0009576523046803073, 1.9999999999997706]
 [-0.013756436574222222, 1.999999999952029]
 [-0.07125740456649217, 1.999999998632208]
 [-0.2589579904135334, 1.9999999770428876]
 [-0.47000019019459244, 1.9999998853401242]
 [-0.6175523056172345, 1.9999996251157426]
 [-0.6604871146338989, 1.9999991687633294]
 [-0.6663384335769652, 1.9999983638263577]
 [1.31463273621472, -1.4502216551864824]
 [1.3246922387276845, -1.446337796343032]
 [1.3345752830424376, -1.4425309909553559]
  [1.3448465813800377, \ -1.4386953334012647] \\
 [1.3549410211470798, -1.4349369320413436]
 [1.3654276856618028, -1.4311498787918024]
 [1.3733682763660415, -1.4282794815915139]
 [1.3815556337247796, -1.4253921223642028]
 [1.398416750766739, -1.4195651966043268]
sol = solve(prob,ARKODE(order=3),abstol=1e-4,reltol=1e-1);
retcode: Success
Interpolation: 3rd order Hermite
t: 262-element Array{Float64,1}:
0.0
5.749667114830345e-12
 4.3901876795072515e-9
8.774625691899672e-9
9.646338593974809e-8
 1.841521461875965e-7
7.700816631708706e-7
 1.3560111801541447e-6
 3.949082228420566e-6
 1.1789802601654659e-5
0.11298197509967592
 0.11298380839542997
 0.11298801005740239
 0.1130053748623104
 0.1131068224569597
 0.11433905890366199
 0.12119409782603513
 0.12662926080921935
 0.12663568109568174
u: 262-element Array{Array{Float64,1},1}:
 [0.0, 2.0]
 [-1.1499235054215125e-5, 2.0]
 [-0.008722807633947647, 1.9999999999808107]
 [-0.017320283728176792, 1.9999999999236775]
 [-0.16757381900079926, 1.9999999915490156]
 [-0.28305989381061913, 1.9999999715852004]
 [-0.6105196086599589, 1.9999996901187271]
 [-0.65844900423416, 1.9999993154753626]
 [-0.6677400989652668, 1.9999975898561386]
 [-0.6666234193152477, 1.9999923623151088]
```

```
[-0.6818868924599188, 1.9221363875991244]
 [-0.7175603752686264, 1.9221350930981596]
 [-0.712803222902284, 1.9221320941669187]
 [-0.7133631481534175, 1.9221197074757677]
 [-0.7133326089415061, 1.922047338705792]
 [-0.7071666434643885, 1.9211679276051756]
 [-0.7375313167127185, 1.9162628557567793]
 [0.24636917387811208, 1.9123576832843268]
 [0.24636917387811208, 1.9123576832843268]
sol = solve(prob,ARKODE(nonlinear convergence coefficient =
1e-6, order=3), abstol=1e-4, reltol=1e-1);
retcode: Success
Interpolation: 3rd order Hermite
t: 5849-element Array{Float64,1}:
5.749667114830345e-12
4.3901876795072515e-9
8.774625691899672e-9
9.646338593974809e-8
1.841521461875965e-7
7.700815831447913e-7
1.3560110201019861e-6
3.949079826682415e-6
 1.1785229199359805e-5
6.282153578661474
6.283343340084043
6.286562194011398
6.289781047938753
6.292335785954065
6.294890523969377
6.296167892977032
6.297445261984688
u: 5849-element Array{Array{Float64,1},1}:
 [0.0, 2.0]
 [-1.1499235054215125e-5, 2.0]
 [-0.008722807633947647, 1.9999999999808107]
 [-0.01732028372817669, 1.9999999999236775]
 [-0.16757381900079918, 1.9999999915490156]
 [-0.28305989360558576, 1.9999999715852004]
 [-0.6105195898251164, 1.9999996901187744]
 [-0.6584488623090199, 1.999999315475422]
 [-0.6677348327309324, 1.9999975898559847]
 [-0.6665784454943076, 1.9999923653490723]
 [1.3318769391697618, -1.4435658592987184]
 [1.3360266395151414, -1.4419787997768507]
 [1.347573057047653, -1.4376598665968587]
 [1.3596736863373744, -1.4333033095612036]
 [1.369063223433025, -1.4298181052243777]
 [1.3790273626823555, -1.4263079600463464]
 [1.3840116143289856, -1.4245433523377944]
 [1.3890441690934623, -1.4227722880905949]
 [1.3994026774014128, -1.4192104815018525]
```

```
sol = solve(prob,ARKODE(order=5,nonlinear convergence coefficient =
1e-3),abstol=1e-4,reltol=1e-1);
retcode: Success
Interpolation: 3rd order Hermite
t: 175-element Array{Float64,1}:
5.749667114830345e-12
 1.6131539822097798e-10
 1.4178810016692538e-9
1.9467016298640084e-8
2.2299839492837688e-7
 6.9410258452898e-7
2.2343380286801016e-6
 4.996464072410812e-6
 1.3177719769063345e-5
 0.21781440165467003
 0.2199025533902211
 0.22199070512577218
 0.22641165376385933
0.2295696852409037
0.2327277167179481
0.23588574819499247
0.2386710571263909
0.23867462686395108
u: 175-element Array{Array{Float64,1},1}:
 [0.0, 2.0]
 [-1.1499235054215124e-5, 2.0]
 [-0.00032255274106088755, 1.999999999999738]
 [-0.0028297393861135135, 1.999999999999992]
 [-0.037818950965746286, 1.9999999996283053]
 [-0.32518303725581216, 1.9999999597287481]
 [-0.5835225092949149, 1.9999997317724212]
 [-0.6654167656320736, 1.9999987322462425]
 [-0.6666680892850902, 1.9999968912426307]
 [-0.6666946561472832, 1.999991437054497]
 [-0.8724519534359474, 1.8446221534793241]
 [-0.7681927666028643, 1.8430177005846022]
 [-0.5135909560385096, 1.8414105680077564]
 [-0.7892024587340847, 1.8379992706417554]
 [-0.7635853085669171, 1.835555634927881]
 [-0.47912592902732515, 1.8331058448058228]
 [-0.7822581531401638, 1.830649920805241]
 [0.034396436491437865, 1.8284785522385856]
 [0.034396436491437865, 1.8284785522385856]
sol = solve(prob,ARKODE(order=5,nonlinear_convergence_coefficient =
1e-4),abstol=1e-4,reltol=1e-1);
retcode: Success
Interpolation: 3rd order Hermite
t: 1618-element Array{Float64,1}:
5.749667114830345e-12
 1.6131539822097798e-10
 1.4178810016692538e-9
```

```
1.9467016298640084e-8
 2.2299839492837688e-7
6.9410258452898e-7
2.2343380286801016e-6
4.996413060669436e-6
 1.3190337112605003e-5
6.2178735057716334
6.223969302456617
6.230065099141601
6.242805651978197
 6.255546204814793
 6.268286757651389
6.2810273104879855
6.2937678633245815
6.3
u: 1618-element Array{Array{Float64,1},1}:
 [0.0, 2.0]
 [-1.1499235054215124e-5, 2.0]
 [-0.00032255274106088755, 1.999999999999738]
 [-0.0028297393861135135, 1.999999999999992]
 [-0.037818950965746286, 1.9999999996283053]
 [-0.32518303725581216, 1.9999999597287481]
 [-0.5835225092949149, 1.9999997317724212]
 [-0.6654163435076001, 1.999998732246102]
 [-0.666668908436716, 1.999996891276912]
 [-0.6666946904177468, 1.9999914286428866]
 [1.1773599643774835, -1.5229500929729562]
 [1.1694104058742847, -1.5158725416037377]
 [1.1880494417611729, -1.5087098220173893]
 [1.2167569401714096, -1.4934498951780604]
 [1.2923315120460783, -1.4777690051239414]
 [1.2227371473134858, -1.4616291764474012]
 [1.3507951884062508, -1.444976089177088]
  [1.4624653585712566, \ -1.4277643260539639] \\
 [1.3983693066218381, -1.4191207815330689]
Additionally, the ROCK methods do not perform well on this benchmark.
setups = [
          #Dict(:alg=>ROCK2())
                                  #Unstable
          #Dict(:alg=>ROCK4())
                                  #needs more iterations
          #Dict(:alq=>ESERK5()),
          ٦
O-element Array{Any,1}
Some of the bad Rosenbrocks fail:
setups = [
  #Dict(:alg=>Hairer4()),
  #Dict(:alg=>Hairer42()),
  #Dict(:alg=>Cash4()),
1
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));
Error: InexactError: trunc(Int64, Inf)
```

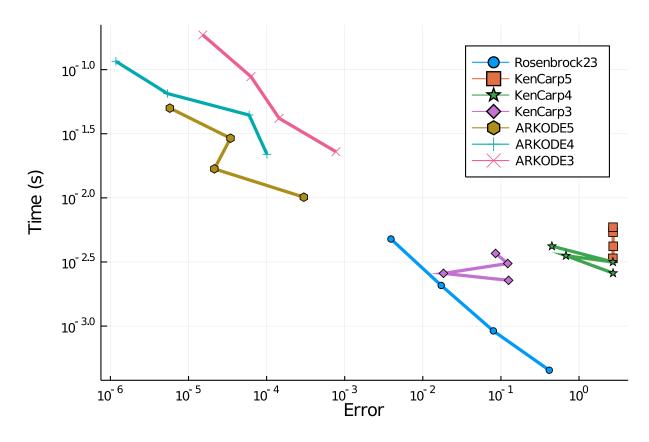
0.2 Low Order and High Tolerance

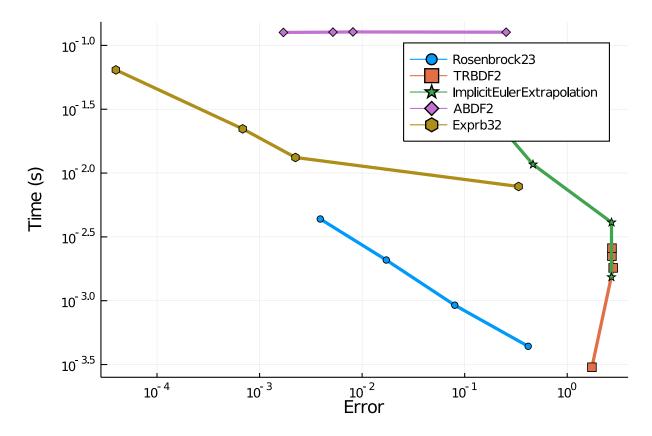
This tests the case where accuracy is not needed as much and quick robust solutions are necessary. Note that ARKODE's convergence coefficient must be lowered to 1e-7 in order to converge.

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())]
Error: UndefVarError: Isoda not defined
wp = WorkPrecisionSet(prob,abstols,reltols,setups;
                      save_everystep=false,appxsol=test_sol,maxiters=Int(1e5),seconds=5)
plot(wp)
Error: ArgumentError: At least one finite value must be provided to formatt
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()),
Error: UndefVarError: lsoda not defined
wp = WorkPrecisionSet(prob,abstols,reltols,setups;
                      save everystep=false,appxsol=test sol,maxiters=Int(1e5),numruns=10)
plot(wp)
```

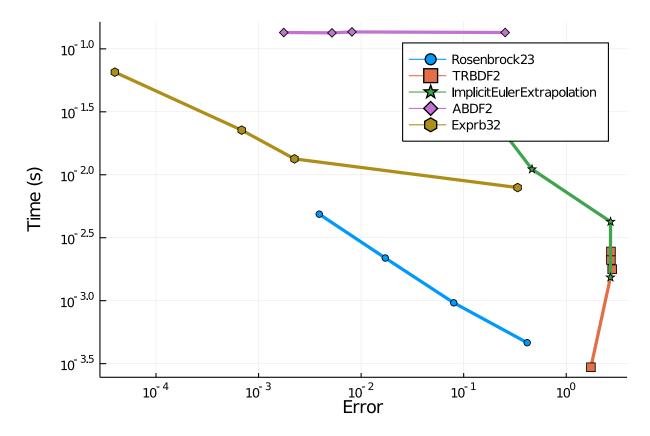
```
Error: ArgumentError: At least one finite value must be provided to formatt
setups = [Dict(:alg=>Rosenbrock23()),
         Dict(:alg=>Kvaerno3()),
          Dict(:alg=>KenCarp4()),
          Dict(:alg=>TRBDF2()),
          Dict(:alg=>KenCarp3()),
          Dict(:alg=>ARKODE(nonlinear_convergence_coefficient = 1e-6)),
          Dict(:alg=>SDIRK2()),
          Dict(:alg=>radau())]
names = ["Rosenbrock23" "Kvaerno3" "KenCarp4" "TRBDF2" "KenCarp3" "ARKODE" "SDIRK2"
wp = WorkPrecisionSet(prob,abstols,reltols,setups;
names=names,save_everystep=false,appxsol=test_sol,maxiters=Int(1e5),seconds=5)
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: ArgumentError: At least one finite value must be provided to formatt
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)
```



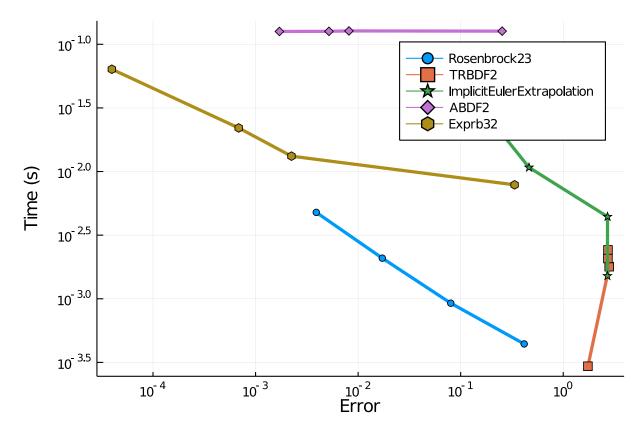


Notice that KenCarp4 is the same overarching algorithm as ARKODE here (with major differences to stage predictors and adaptivity though). In this case, KenCarp4 is more robust and more efficient than ARKODE. CVODE_BDF does quite well here, which is unusual for it on small equations. You can see that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

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

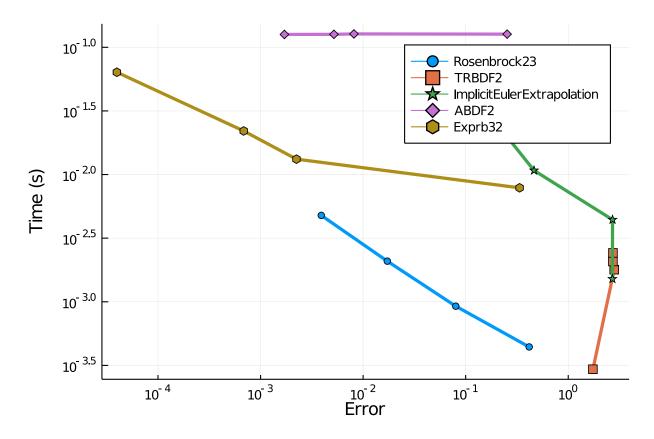


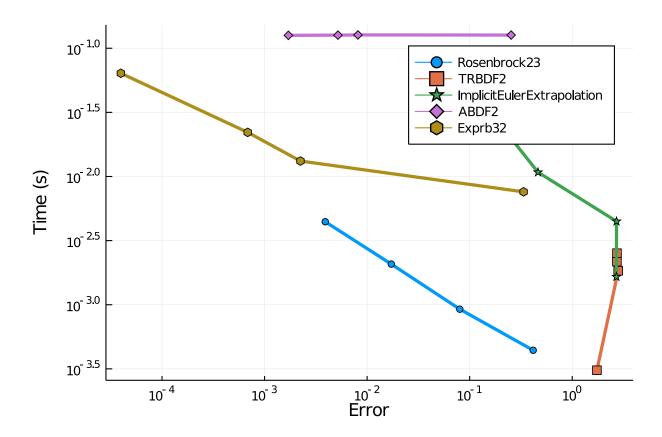
Error: UndefVarError: lsoda not defined



names=names,appxsol=test_sol,maxiters=Int(1e5),error_estimator=:12,seconds=5)

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.

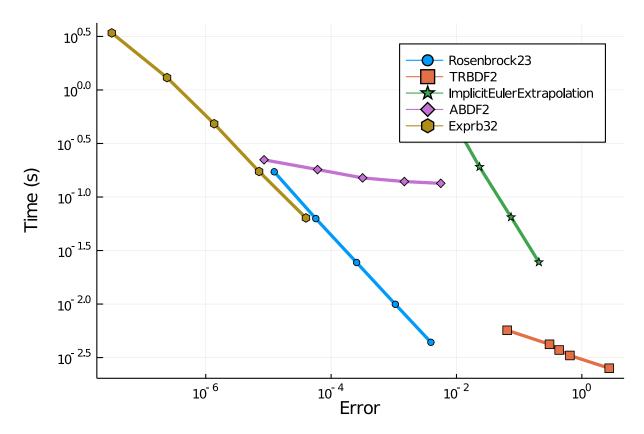




0.2.1 Higher accuracy tests

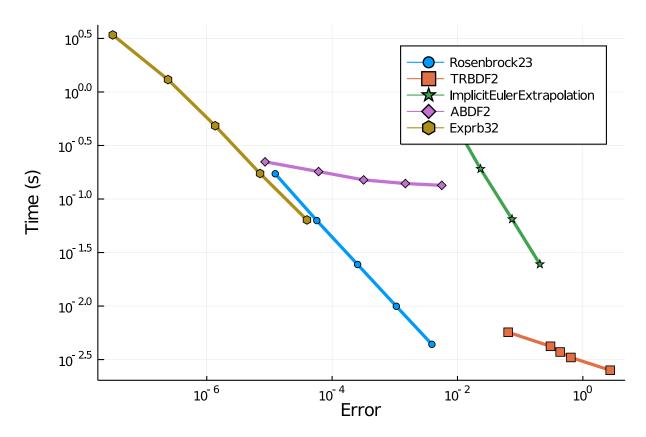
abstols = 1.0 ./ 10.0 .^ (7:11)

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

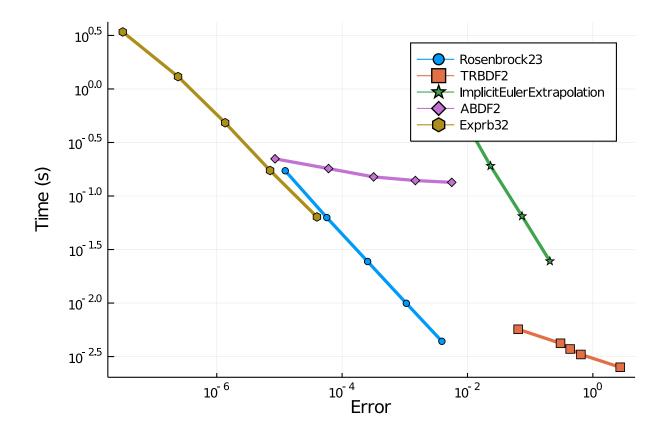


 $names=names, save_everystep=false, appxsol=test_sol, maxiters=Int(1e6), seconds=5)$

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 ODEInterface.help_install.

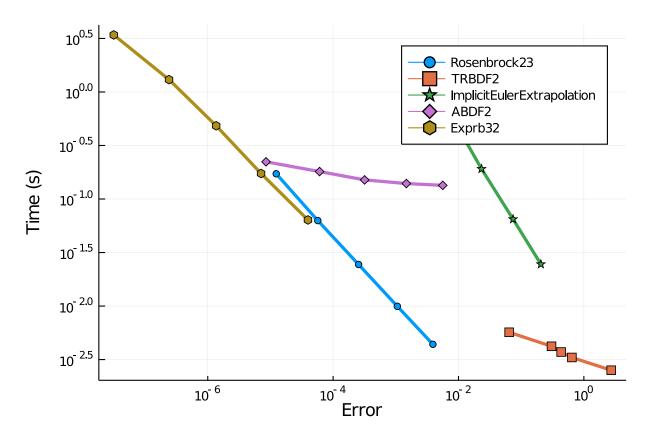


Error: Cannot find method(s) for radau! I've tried to loadODESolvers(), but it didn't work. Please check ODEInterface.help_solversupport() and call lo adODESolvers and check also this output. For further information see also O DEInterface.help_install.



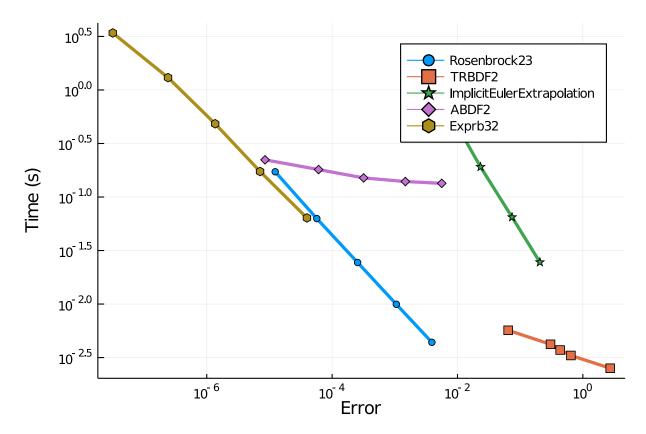
Error: UndefVarError: lsoda not defined

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.

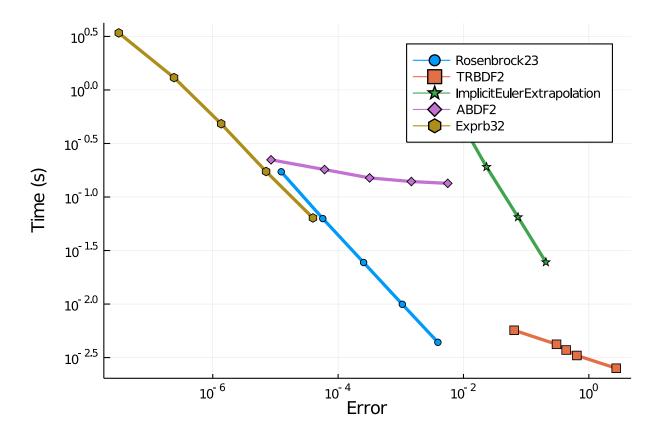


Error: Cannot find method(s) for radau! I've tried to loadODESolvers(), but it didn't work. Please check ODEInterface.help_solversupport() and call lo adODESolvers and check also this output. For further information see also O DEInterface.help_install.

names=names,appxsol=test_sol,maxiters=Int(1e6),error_estimate=:12,seconds=5)



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 ODEInterface.help_install.



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.

```
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/JuliaDi

To locally run this tutorial, do the following commands:

DiffEqBenchmarks.weave file("StiffODE", "VanDerPol.jmd")

using DiffEqBenchmarks

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