VanDerPol Work-Precision Diagrams

Chris Rackauckas

July 21, 2020

```
using OrdinaryDiffEq, DiffEqDevTools, Sundials, ParameterizedFunctions, Plots, ODE,
ODEInterfaceDiffEq, ODEInterface, LSODA
```

```
Error: Failed to precompile OrdinaryDiffEq [1dea7af3-3e70-54e6-95c3-0bf5283
fa5ed] to /builds/JuliaGPU/DiffEqBenchmarks.jl/.julia/compiled/v1.4/Ordinar
yDiffEq/DlSvy_YAMOL.ji.
```

```
gr()
```

```
Error: UndefVarError: gr not defined
```

```
using LinearAlgebra
LinearAlgebra.BLAS.set_num_threads(1)
```

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

```
Error: LoadError: UndefVarError: @ode_def not defined
in expression starting at none:2
```

```
prob = ODEProblem(van,[0;2.],(0.0,6.3),1e6)
```

```
Error: UndefVarError: ODEProblem not defined
```

```
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)
```

```
Error: UndefVarError: CVODE_BDF not defined
```

```
test_sol = TestSolution(sol)
```

```
Error: UndefVarError: TestSolution not defined
```

0.0.1 Plot Test

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

```
Error: UndefVarError: plot not defined
```

```
plot(sol)
```

```
Error: UndefVarError: plot not defined
```

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);
```

```
Error: UndefVarError: ARKODE not defined
```

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

```
Error: UndefVarError: ARKODE not defined
```

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

```
Error: UndefVarError: ARKODE not defined
```

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

```
Error: UndefVarError: ARKODE not defined
```

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

```
Error: UndefVarError: ARKODE not defined
```

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

```
Error: UndefVarError: ARKODE not defined
```

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()),
          ]
```

```
0-element Array{Any,1}
```

Some of the bad Rosenbrocks fail:

```
setups = [
  #Dict(:alg=>Hairer4()),
  #Dict(:alg=>Hairer42()),
  #Dict(:alg=>Cash4()),
]
```

```
0-element Array{Any,1}
```

The EPIRK and exponential methods also fail:

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

```
Error: UndefVarError: EXPRB53s3 not defined
```

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

```
Error: UndefVarError: EPIRK4s3B not defined
```

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

```
Error: UndefVarError: EPIRK5P2 not defined
```

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: Rosenbrock23 not defined
```

```
wp = WorkPrecisionSet(prob,abstols,reltols,setups;
                      save_everystep=false,appxsol=test_sol,maxiters=Int(1e5),seconds=5)
```

```
Error: UndefVarError: test_sol not defined
```

```
plot(wp)
```

```
Error: UndefVarError: plot not defined
```

```
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: Rosenbrock23 not defined
```

```
gr()
```

```
Error: UndefVarError: gr not defined
```

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

```
Error: UndefVarError: test_sol not defined
```

```
plot(wp)
```

```
Error: UndefVarError: plot not defined
```

```
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())]
```

```
Error: UndefVarError: Rosenbrock23 not defined
```

```
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)
```

```
Error: UndefVarError: test_sol not defined
```

```
plot(wp)
```

```
Error: UndefVarError: plot not defined
```

```
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))]
```

```
Error: UndefVarError: Rosenbrock23 not defined
```

```
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)

Error: UndefVarError: test_sol not defined

plot(wp)

Error: UndefVarError: plot not defined

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()),
]

Error: UndefVarError: Rosenbrock23 not defined

wp = WorkPrecisionSet(prob,abstols,reltols,setups;
                      save_everystep=false,appxsol=test_sol,maxiters=Int(1e5),numruns=10)

Error: UndefVarError: test_sol not defined

plot(wp)

Error: UndefVarError: plot not defined
```

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())]

Error: UndefVarError: Rosenbrock23 not defined

wp = WorkPrecisionSet(prob,abstols,reltols,setups;
                      error_estimator=:l2,appxsol=test_sol,maxiters=Int(1e5),seconds=5)

Error: UndefVarError: test_sol not defined
```

```
plot(wp)
```

```
Error: UndefVarError: plot not defined
```

```
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: Rosenbrock23 not defined
```

```
gr()
```

```
Error: UndefVarError: gr not defined
```

```
wp = WorkPrecisionSet(prob,abstols,reltols,setups;error_estimator=:l2,
                      save_everystep=false,appxsol=test_sol,maxiters=Int(1e5),numruns=10)
```

```
Error: UndefVarError: test_sol not defined
```

```
plot(wp)
```

```
Error: UndefVarError: plot not defined
```

```
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())]
```

```
Error: UndefVarError: Rosenbrock23 not defined
```

```
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)
```

```
Error: UndefVarError: test_sol not defined
```

```
plot(wp)
```

```
Error: UndefVarError: plot not defined
```

```
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()),
]
```

```
Error: UndefVarError: Rosenbrock23 not defined
```

```
wp = WorkPrecisionSet(prob,abstols,reltols,setups;error_estimator=:l2,
                      save_everystep=false,appxsol=test_sol,maxiters=Int(1e5),numruns=10)
```

```
Error: UndefVarError: test_sol not defined
```

```
plot(wp)
```

```
Error: UndefVarError: plot not defined
```

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())]
```

```
Error: UndefVarError: Rodas3 not defined
```

```
wp = WorkPrecisionSet(prob,abstols,reltols,setups;
                      save_everystep=false,appxsol=test_sol,maxiters=Int(1e6),seconds=5)
```

```
Error: UndefVarError: test_sol not defined
```

```
plot(wp)
```

```
Error: UndefVarError: plot not defined
```

```
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())]
```

```
Error: UndefVarError: Rodas3 not defined
```

```
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)
```

```
Error: UndefVarError: test_sol not defined
```

```
plot(wp)
```

```
Error: UndefVarError: plot not defined
```

```
setups = [Dict(:alg=>Rodas3()),
          Dict(:alg=>CVODE_BDF()),
          Dict(:alg=>Rodas4()),
          Dict(:alg=>radau()),
          Dict(:alg=>Rodas5())]
```

```
Error: UndefVarError: Rodas3 not defined
```

```
wp = WorkPrecisionSet(prob,abstols,reltols,setups;
                      save_everystep=false,appxsol=test_sol,maxiters=Int(1e6),seconds=5)
```

```
Error: UndefVarError: test_sol not defined
```

```
plot(wp)
```

```
Error: UndefVarError: plot not defined
```

```
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())]
```

```
Error: UndefVarError: Rodas3 not defined
```

```
wp = WorkPrecisionSet(prob,abstols,reltols,setups;error_estimate=:l2,
                      save_everystep=false,appxsol=test_sol,maxiters=Int(1e6),seconds=5)
```

```
Error: UndefVarError: test_sol not defined
```

```
plot(wp)
```

```
Error: UndefVarError: plot not defined
```

```
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())]
```

```
Error: UndefVarError: Rodas3 not defined
```

```
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)

Error: UndefVarError: test_sol not defined

plot(wp)

Error: UndefVarError: plot not defined

setups = [Dict(:alg=>CVODE_BDF()),
          Dict(:alg=>Rodas4()),
          Dict(:alg=>radau()),
          Dict(:alg=>Rodas5())]

Error: UndefVarError: CVODE_BDF not defined

wp = WorkPrecisionSet(prob,abstols,reltols,setups;
                      appxsol=test_sol,maxiters=Int(1e6),error_estimate=:l2,seconds=5)

Error: UndefVarError: test_sol not defined

plot(wp)

Error: UndefVarError: plot not defined
```

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 SciMLBenchmarks
SciMLBenchmarks.bench_footer(WEAVE_ARGS[:folder],WEAVE_ARGS[:file])
```

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("StiffODE","VanDerPol.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 = 8
```

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 2.24.0
[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 5.4.0
[91a5bcdd-55d7-5caf-9e0b-520d859cae80] Plots 1.5.5
[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
```