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 = \mu * ((1-x^2)*y - x)
  dx = 1*y
end \mu
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)
```

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
# 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(:alq=>ROCK2())
                                  #Unstable
          #Dict(:alg=>ROCK4())
                                  #needs more iterations
          #Dict(:alq=>ESERK5()),
O-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.

```
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;
\verb|names=names|, \verb|save_every| step= false, \verb|appxsol=test_sol|, \verb|maxiters=Int(1e5)|, \verb|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.

```
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=:12,
                      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=:12,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()),
٦
```

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=:12,
                      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=:12,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=:12,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

using SciMLBenchmarks

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:

```
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_LOAD_PATH = /builds/JuliaGPU/DiffEqBenchmarks.jl:
  JULIA DEPOT PATH = /builds/JuliaGPU/DiffEqBenchmarks.jl/.julia
  JULIA_CUDA_MEMORY_LIMIT = 2147483648
  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
```