ROBER Work-Precision Diagrams

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```
using OrdinaryDiffEq, DiffEqDevTools, Sundials, ParameterizedFunctions, Plots, ODE,
ODEInterfaceDiffEq, 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)
```

```
rober = @ode_def begin
  dy_1 = -k_1*y_1+k_3*y_2*y_3
  dy_2 =  k_1*y_1-k_2*y_2^2-k_3*y_2*y_3
  dy_3 =  k_2*y_2^2
end k_1 k_2 k_3
```

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

```
prob = ODEProblem(rober,[1.0,0.0,0.0],(0.0,1e5),(0.04,3e7,1e4))
```

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

```
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
```

```
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,labels=["y1","y2","y3"])
```

```
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=1/10)
#catch e
#    println(e)
#end
```

`ARKODE` needs a lower `nonlinear_convergence_coefficient` in order to not diverge.

```
#sol = solve(prob,ARKODE(nonlinear_convergence_coefficient =
1e-6),abstol=1e-5,reltol=1e-1); # Noisy, output omitted

sol = solve(prob,ARKODE(nonlinear_convergence_coefficient =
1e-7),abstol=1e-5,reltol=1e-1);
```

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

Note that `1e-7` matches the value from the Sundials manual which was required for their example to converge on this problem. The default is `1e-1`.

```
#sol = solve(prob,ARKODE(order=3),abstol=1e-4,reltol=1e-1); # Fails to diverge but
doesn't finish

#sol = solve(prob,ARKODE(order=5),abstol=1e-4,reltol=1e-1); # Noisy, output omitted

#sol = solve(prob,ARKODE(order=5,nonlinear_convergence_coefficient =
1e-9),abstol=1e-5,reltol=1e-1); # Noisy, output omitted
```

Additionally, the ROCK methods do not perform well on this benchmark.

```
setups = [
          #Dict(:alg=>ROCK2())    #Unstable
          #Dict(:alg=>ROCK4())    #needs more iterations
          ]
```

```
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
```

PDIRK44 also fails

```
sol = solve(prob,PDIRK44(),dt=2.0^(-8));
```

```
Error: UndefVarError: PDIRK44 not defined
```

In fact, all non-adaptive methods fail on this problem.

0.2 High Tolerances

This is the speed when you just want the answer. `ode23s` from ODE.jl was removed since it fails. Note that at high tolerances Sundials' `CVODE_BDF` fails as well so it's excluded from this test.

```
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=>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=>SDIRK2()), # Removed because it's bad
          Dict(:alg=>radau())]
```

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

```
names = ["Rosenbrock23" "Kvaerno3" "KenCarp4" "TRBDF2" "KenCarp3" "radau"]
wp = WorkPrecisionSet(prob,abstols,reltols,setups;names=names,
                      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=>KenCarp5()),
          Dict(:alg=>KenCarp4()),
          Dict(:alg=>KenCarp3()),
          Dict(:alg=>ARKODE(nonlinear_convergence_coefficient = 1e-9,order=5)),
          Dict(:alg=>ARKODE(nonlinear_convergence_coefficient = 1e-8)),
          Dict(:alg=>ARKODE(nonlinear_convergence_coefficient = 1e-7,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),numruns=10)
```

```
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()), # Maxiters
          Dict(:alg=>QNDF()),
          Dict(:alg=>Exprb43()),
          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
```

0.2.1 Timeseries Errors

```
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=>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_estimate=: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()),
          Dict(:alg=>Kvaerno3()),
          Dict(:alg=>KenCarp4()),
          Dict(:alg=>TRBDF2()),
          Dict(:alg=>KenCarp3()),
    # Dict(:alg=>SDIRK2()), # Removed because it's bad
          Dict(:alg=>radau())]
```

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

```
names = ["Rosenbrock23" "Kvaerno3" "KenCarp4" "TRBDF2" "KenCarp3" "radau"]
wp = WorkPrecisionSet(prob,abstols,reltols,setups;names=names,
                      appxsol=test_sol,maxiters=Int(1e5),error_estimate=:l2,numruns=10)
```

```
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()), # Maxiters
          Dict(:alg=>QNDF()),
          Dict(:alg=>Exprb43()),
          Dict(:alg=>Exprb32()),
]
```

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

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

0.2.2 Low Tolerances

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

```
abstols = 1.0 ./ 10.0 .^ (7:12)
reltols = 1.0 ./ 10.0 .^ (4:9)

setups = [Dict(:alg=>Rodas5()),
          Dict(:alg=>Rodas4P()),
          Dict(:alg=>CVODE_BDF()),
          Dict(:alg=>ddebdf()),
          Dict(:alg=>Rodas4()),
          Dict(:alg=>rodas()),
          Dict(:alg=>lsoda()),
          Dict(:alg=>radau()),
          Dict(:alg=>RadauIIA5()),
]
```

```
Error: UndefVarError: Rodas5 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=>Rodas4P()),
          Dict(:alg=>Kvaerno4()),
          Dict(:alg=>Kvaerno5()),
          Dict(:alg=>CVODE_BDF()),
          Dict(:alg=>KenCarp4()),
          Dict(:alg=>KenCarp5()),
          Dict(:alg=>Rodas4()),
          Dict(:alg=>Rodas5()),
          Dict(:alg=>radau())]
```

```
Error: UndefVarError: Rodas4P 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
```

```
abstols = 1.0 ./ 10.0 .^ (10:12)
reltols = 1.0 ./ 10.0 .^ (7:9)

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

Error: UndefVarError: Rodas4 not defined

names = ["Rodas4" "Rodas5"]
wp = WorkPrecisionSet(prob,abstols,reltols,setups;names=names,
                      save_everystep=false,appxsol=test_sol,maxiters=Int(1e5),numruns=10)

Error: UndefVarError: test_sol not defined

plot(wp)

Error: UndefVarError: plot not defined
```

0.2.3 Conclusion

At high tolerances, `Rosenbrock23` and `lsoda` hit the the error estimates and are fast. At lower tolerances and normal user tolerances, `Rodas4` and `Rodas5` are extremely fast. `lsoda` does quite well across both ends. When you get down to `reltol=1e-9` `radau` begins to become as efficient as `Rodas4`, and it continues to do well below that.

```
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","ROBER.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
```