OREGO Work-Precision Diagrams

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July 21, 2020

```
using OrdinaryDiffEq, DiffEqDevTools, ParameterizedFunctions, Plots, ODE,
ODEInterfaceDiffEq, LSODA, Sundials
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() #gr(fmt=:png)
Error: UndefVarError: gr not defined
using LinearAlgebra
LinearAlgebra.BLAS.set_num_threads(1)
f = @ode_def Orego begin
 dy1 = p1*(y2+y1*(1-p2*y1-y2))
 dy2 = (y3-(1+y1)*y2)/p1
 dy3 = p3*(y1-y3)
end p1 p2 p3
Error: LoadError: UndefVarError: @ode_def not defined
in expression starting at none:2
p = [77.27, 8.375e-6, 0.161]
prob = ODEProblem(f,[1.0,2.0,3.0],(0.0,30.0),p)
Error: UndefVarError: ODEProblem not defined
sol = solve(prob,Rodas5(),abstol=1/10^14,reltol=1/10^14)
Error: UndefVarError: Rodas5 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_prob = ODEProblem(f,[1.0,2.0,3.0],(0.0,400.0),p)
Error: UndefVarError: ODEProblem not defined
sol = solve(plot_prob,CVODE_BDF())
Error: UndefVarError: CVODE_BDF not defined
plot(sol,yscale=:log10)
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
# sol = solve(prob, GIRadIIA3(), dt=1/10)
#catch e
# println(e)
#end
sol = solve(prob, ARKODE(), abstol=1e-5, reltol=1e-1);
Error: UndefVarError: ARKODE not defined
sol = solve(prob, ARKODE(nonlinear_convergence_coefficient =
1e-3),abstol=1e-5,reltol=1e-1);
Error: UndefVarError: ARKODE not defined
sol = solve(prob, ARKODE(order=3), abstol=1e-5, reltol=1e-1);
Error: UndefVarError: ARKODE not defined
sol = solve(prob, ARKODE(order=3, nonlinear_convergence_coefficient =
1e-5),abstol=1e-5,reltol=1e-1);
Error: UndefVarError: ARKODE not defined
sol = solve(prob, ARKODE(order=5), abstol=1e-5, reltol=1e-1);
Error: UndefVarError: ARKODE not defined
```

The stabilized explicit methods are not stable enough to handle this problem well. While they don't diverge, they are really slow.

```
setups = [
    #Dict(:alg=>ROCK2()) #Unstable
    #Dict(:alg=>ROCK4()) #needs more iterations
    #Dict(:alg=>ESERK5()),
]
```

```
O-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
     High Tolerances
0.2
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=>RadauIIA5()),
          Dict(:alg=>ROS34PW1a()),
          Dict(:alg=>lsoda()),
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
wp = WorkPrecisionSet(prob,abstols,reltols,setups;dense = false,verbose=false,
                      appxsol=test_sol,maxiters=Int(1e5),error_estimate=:12,numruns=10)
Error: UndefVarError: test sol not defined
plot(wp)
```

Error: UndefVarError: plot not defined

```
wp = WorkPrecisionSet(prob,abstols,reltols,setups;
                      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=>Kvaerno3()),
          Dict(:alg=>CVODE_BDF()),
          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
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
wp = WorkPrecisionSet(prob, abstols, reltols, setups; dense = false, verbose = false,
                      appxsol=test_sol,maxiters=Int(1e5),error_estimate=:12,numruns=10)
Error: UndefVarError: test_sol not defined
plot(wp)
Error: UndefVarError: plot not defined
wp = WorkPrecisionSet(prob,abstols,reltols,setups;
                      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=>KenCarp5()),
          Dict(:alg=>KenCarp4()),
          Dict(:alg=>KenCarp3()),
          Dict(:alg=>ARKODE(order=5)),
          Dict(:alg=>ARKODE(nonlinear_convergence_coefficient = 1e-6)),
          Dict(:alg=>ARKODE(nonlinear_convergence_coefficient = 1e-5,order=3))
          1
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()),
          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 Low Tolerances
This is the speed at lower tolerances, measuring what's good when accuracy is needed.
abstols = 1.0 ./ 10.0 .^ (7:13)
reltols = 1.0 ./ 10.0 .^ (4:10)
setups = [Dict(:alg=>GRK4A()),
          Dict(:alg=>Rodas4P()),
          Dict(:alg=>CVODE BDF()),
          Dict(:alg=>ddebdf()),
          Dict(:alg=>Rodas4()),
          Dict(:alg=>rodas()),
          Dict(:alg=>radau()),
          Dict(:alg=>RadauIIA5()),
          Dict(:alg=>lsoda()),
]
Error: UndefVarError: GRK4A not defined
```

save_everystep=false,appxsol=test_sol,maxiters=Int(1e5),numruns=10)

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

Error: UndefVarError: test_sol not defined

plot(wp)

```
Error: UndefVarError: plot not defined
wp = WorkPrecisionSet(prob,abstols,reltols,setups;verbose=false,
dense=false,appxsol=test_sol,maxiters=Int(1e5),error_estimate=:12,numruns=10)
Error: UndefVarError: test_sol not defined
plot(wp)
Error: UndefVarError: plot not defined
wp = WorkPrecisionSet(prob,abstols,reltols,setups;
                      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=>Rodas5()),
          Dict(:alg=>Kvaerno5());
          Dict(:alg=>CVODE_BDF()),
          Dict(:alg=>KenCarp4()),
          Dict(:alg=>KenCarp5()),
          Dict(:alg=>Rodas4()),
          Dict(:alg=>radau())]
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
wp = WorkPrecisionSet(prob,abstols,reltols,setups;verbose=false,
dense=false,appxsol=test_sol,maxiters=Int(1e5),error_estimate=:12,numruns=10)
Error: UndefVarError: test_sol not defined
plot(wp)
Error: UndefVarError: plot not defined
wp = WorkPrecisionSet(prob,abstols,reltols,setups;
                      appxsol=test_sol,maxiters=Int(1e5),error_estimate=:L2,numruns=10)
Error: UndefVarError: test sol not defined
plot(wp)
Error: UndefVarError: plot not defined
```

The following algorithms were removed since they failed.

0.2.2 Conclusion

At high tolerances, Rosenbrock23 hits the the error estimates and is fast. At lower tolerances and normal user tolerances, Rodas4 and Rodas5 are extremely fast. 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","Orego.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-838fccc9c8e] LinearAlgebra
```