HIRES Work-Precision Diagrams

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```
using OrdinaryDiffEq, ParameterizedFunctions, Plots, ODE, ODEInterfaceDiffEq, LSODA,
DiffEqDevTools, 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.
using LinearAlgebra
LinearAlgebra.BLAS.set_num_threads(1)
gr() #gr(fmt=:png)
Error: UndefVarError: gr not defined
f = @ode_def Hires begin
  dy1 = -1.71*y1 + 0.43*y2 + 8.32*y3 + 0.0007
  dy2 = 1.71*y1 - 8.75*y2
  dy3 = -10.03*y3 + 0.43*y4 + 0.035*y5
  dy4 = 8.32*y2 + 1.71*y3 - 1.12*y4
  dy5 = -1.745*y5 + 0.43*y6 + 0.43*y7
  dy6 = -280.0*y6*y8 + 0.69*y4 + 1.71*y5 -
          0.43*y6 + 0.69*y7
 dy7 = 280.0*y6*y8 - 1.81*y7
  dy8 = -280.0*y6*y8 + 1.81*y7
Error: LoadError: UndefVarError: @ode_def not defined
in expression starting at none:2
u0 = zeros(8)
u0[1] = 1
u0[8] = 0.0057
prob = ODEProblem(f,u0,(0.0,321.8122))
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(sol)

Error: UndefVarError: plot not defined
plot(sol,tspan=(0.0,5.0))

Error: UndefVarError: plot not defined
```

0.1 Omissions

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
```

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()),
#Dict(:alg=>ROCK4())
#Dict(:alg=>ESERK5())
]
O-element Array{Any,1}
```

0.2 High Tolerances

This is the speed when you just want the answer.

```
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)
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)
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))
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)
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)
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()),
          Dict(:alg=>ARKODE(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))
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)
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()),
٦
Error: UndefVarError: Rosenbrock23 not defined
wp = WorkPrecisionSet(prob,abstols,reltols,setups;
                      save_everystep=false,appxsol=test_sol,maxiters=Int(1e5))
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=>Rodas5()),
          Dict(:alg=>rodas()),
          Dict(:alg=>radau()),
          Dict(:alg=>lsoda()),
          Dict(:alg=>RadauIIA5()),
٦
Error: UndefVarError: GRK4A not defined
wp = WorkPrecisionSet(prob,abstols,reltols,setups;
                      save_everystep=false,appxsol=test_sol,maxiters=Int(1e5))
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)
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)
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=>Rodas4()),
          Dict(:alg=>radau())]
Error: UndefVarError: Rodas5 not defined
wp = WorkPrecisionSet(prob,abstols,reltols,setups;
                      save_everystep=false,appxsol=test_sol,maxiters=Int(1e5))
```

```
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)
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)
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()),
          Dict(:alg=>ARKODE(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))
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)
Error: UndefVarError: test_sol not defined
plot(wp)
Error: UndefVarError: plot not defined
The following algorithms were removed since they failed.
#setups = [#Dict(:alg=>Hairer4()),
          #Dict(:alg=>Hairer42()),
          #Dict(:alg=>Rodas3()),
          #Dict(:alg=>Kvaerno4()),
          #Dict(:alg=>KenCarp5()),
          #Dict(:alg=>Cash4())
#7
#wp = WorkPrecisionSet(prob,abstols,reltols,setups;
                       save\_everystep=false, appxsol=test\_sol, maxiters=Int(1e5))
#plot(wp)
```

0.2.2 Conclusion

At high tolerances, Rosenbrock23 and lsoda hits the the error estimates and are fast. At lower tolerances and normal user tolerances, Rodas5 is extremely fast. When you get down to reltol=1e-10 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","Hires.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 = 0.
  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
```