POLLU Work-Precision Diagrams

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July 21, 2020

```
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() # gr(fmt=:png)
```

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

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

const k1=.35e0
const k2=.266e2
const k3=.123e5
const k4=.86e-3
const k5=.82e-3
const k6=.15e5
const k7=.13e-3
const k8=.24e5
const k9=.165e5
const k10=.9e4
const k11=.22e-1
const k12=.12e5
const k13=.188e1
const k14=.163e5
const k15=.48e7
const k16=.35e-3
const k17=.175e-1
const k18=.1e9
const k19=.444e12
const k20=.124e4
const k21=.21e1
const k22=.578e1
const k23=.474e-1
const k24=.178e4
const k25=.312e1

function f(dy,y,p,t)
 r1  = k1 *y[1]
 r2  = k2 *y[2]*y[4]
 r3  = k3 *y[5]*y[2]
 r4  = k4 *y[7]
 r5  = k5 *y[7]
 r6  = k6 *y[7]*y[6]
 r7  = k7 *y[9]
 r8  = k8 *y[9]*y[6]
 r9  = k9 *y[11]*y[2]
 r10 = k10*y[11]*y[1]
 r11 = k11*y[13]
 r12 = k12*y[10]*y[2]
 r13 = k13*y[14]
 r14 = k14*y[1]*y[6]
 r15 = k15*y[3]
 r16 = k16*y[4]
 r17 = k17*y[4]
 r18 = k18*y[16]
 r19 = k19*y[16]
 r20 = k20*y[17]*y[6]
 r21 = k21*y[19]
 r22 = k22*y[19]
 r23 = k23*y[1]*y[4]
 r24 = k24*y[19]*y[1]
 r25 = k25*y[20]

 dy[1]  = -r1-r10-r14-r23-r24+
          r2+r3+r9+r11+r12+r22+r25
 dy[2]  = -r2-r3-r9-r12+r1+r21
 dy[3]  = -r15+r1+r17+r19+r22
 dy[4]  = -r2-r16-r17-r23+r15
 dy[5]  = -r3+r4+r4+r6+r7+r13+r20
 dy[6]  = -r6-r8-r14-r20+r3+r18+r18
 dy[7]  = -r4-r5-r6+r13
 dy[8]  = r4+r5+r6+r7
 dy[9]  = -r7-r8
 dy[10] = -r12+r7+r9
 dy[11] = -r9-r10+r8+r11
 dy[12] = r9
 dy[13] = -r11+r10
 dy[14] = -r13+r12
 dy[15] = r14
 dy[16] = -r18-r19+r16
 dy[17] = -r20
 dy[18] = r20
 dy[19] = -r21-r22-r24+r23+r25
 dy[20] = -r25+r24
end

function fjac(J,y,p,t)
      J .= 0.0
      J[1,1]   = -k1-k10*y[11]-k14*y[6]-k23*y[4]-k24*y[19]
      J[1,11]  = -k10*y[1]+k9*y[2]
      J[1,6]   = -k14*y[1]
      J[1,4]   = -k23*y[1]+k2*y[2]
      J[1,19]  = -k24*y[1]+k22
      J[1,2]   = k2*y[4]+k9*y[11]+k3*y[5]+k12*y[10]
      J[1,13]  = k11
      J[1,20]  = k25
      J[1,5]   = k3*y[2]
      J[1,10]  = k12*y[2]

      J[2,4]   = -k2*y[2]
```

```
J[2,5]   = -k3*y[2]
J[2,11]  = -k9*y[2]
J[2,10]  = -k12*y[2]
J[2,19]  = k21
J[2,1]   = k1
J[2,2]   = -k2*y[4]-k3*y[5]-k9*y[11]-k12*y[10]

J[3,1]   = k1
J[3,4]   = k17
J[3,16]  = k19
J[3,19]  = k22
J[3,3]   = -k15

J[4,4]   = -k2*y[2]-k16-k17-k23*y[1]
J[4,2]   = -k2*y[4]
J[4,1]   = -k23*y[4]
J[4,3]   = k15

J[5,5]   = -k3*y[2]
J[5,2]   = -k3*y[5]
J[5,7]   = 2k4+k6*y[6]
J[5,6]   = k6*y[7]+k20*y[17]
J[5,9]   = k7
J[5,14]  = k13
J[5,17]  = k20*y[6]

J[6,6]   = -k6*y[7]-k8*y[9]-k14*y[1]-k20*y[17]
J[6,7]   = -k6*y[6]
J[6,9]   = -k8*y[6]
J[6,1]   = -k14*y[6]
J[6,17]  = -k20*y[6]
J[6,2]   = k3*y[5]
J[6,5]   = k3*y[2]
J[6,16]  = 2k18

J[7,7]   = -k4-k5-k6*y[6]
J[7,6]   = -k6*y[7]
J[7,14]  = k13

J[8,7]   = k4+k5+k6*y[6]
J[8,6]   = k6*y[7]
J[8,9]   = k7

J[9,9]   = -k7-k8*y[6]
J[9,6]   = -k8*y[9]

J[10,10] = -k12*y[2]
J[10,2]  = -k12*y[10]+k9*y[11]
J[10,9]  = k7
J[10,11] = k9*y[2]

J[11,11] = -k9*y[2]-k10*y[1]
J[11,2]  = -k9*y[11]
J[11,1]  = -k10*y[11]
J[11,9]  = k8*y[6]
J[11,6]  = k8*y[9]
J[11,13] = k11

J[12,11] = k9*y[2]
```

```
    J[12,2]  = k9*y[11]

    J[13,13] = -k11
    J[13,11] = k10*y[1]
    J[13,1]  = k10*y[11]

    J[14,14] = -k13
    J[14,10] = k12*y[2]
    J[14,2]  = k12*y[10]

    J[15,1]  = k14*y[6]
    J[15,6]  = k14*y[1]

    J[16,16] = -k18-k19
    J[16,4]  = k16

    J[17,17] = -k20*y[6]
    J[17,6]  = -k20*y[17]

    J[18,17] = k20*y[6]
    J[18,6]  = k20*y[17]

    J[19,19] = -k21-k22-k24*y[1]
    J[19,1]  = -k24*y[19]+k23*y[4]
    J[19,4]  = k23*y[1]
    J[19,20] = k25

    J[20,20] = -k25
    J[20,1]  = k24*y[19]
    J[20,19] = k24*y[1]

    return
end

u0 = zeros(20)
u0[2]  = 0.2
u0[4]  = 0.04
u0[7]  = 0.1
u0[8]  = 0.3
u0[9]  = 0.01
u0[17] = 0.007
prob = ODEProblem(ODEFunction(f, jac=fjac),u0,(0.0,60.0))
```

```
Error: UndefVarError: ODEFunction 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 fail.

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

```
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 High Tolerances

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=>lsoda()),
          Dict(:alg=>RadauIIA5()),
          ]
```

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

```
wp = WorkPrecisionSet(prob,abstols,reltols,setups;verbose=false,
                      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=:l2,numruns=10)
```

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

```
plot(wp)
```

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

```
wp = WorkPrecisionSet(prob,abstols,reltols,setups;verbose=false,
                      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=>Rodas4()),
          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=:l2,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()),
          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),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))
```

```
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=>lsoda())
          ]
```

```
Error: UndefVarError: GRK4A not defined
```

```
wp = WorkPrecisionSet(prob,abstols,reltols,setups;verbose=false,
                      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=:l2,numruns=10)
```

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

```
plot(wp)
```

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

```
wp = WorkPrecisionSet(prob,abstols,reltols,setups;verbose=false,
                      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=>Kvaerno4()),
          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=:l2,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.

```
#setups = [#Dict(:alg=>Hairer4()),
          #Dict(:alg=>Hairer42()),
          #Dict(:alg=>Rodas3()),
          #Dict(:alg=>Cash4())
#]
#wp = WorkPrecisionSet(prob,abstols,reltols,setups;
#
save_everystep=false,appxsol=test_sol,maxiters=Int(1e5),numruns=10)
#plot(wp)
```

0.2.2 Conclusion

Sundials `CVODE_BDF` the best here. `lsoda` does well at high tolerances but then grows fast when tolerances get too low. `KenCarp4` or `Rodas5` is a decent substitute when necessary.

```
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","Pollution.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
```