BCR Work-Precision Diagrams

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The following benchmark is of a 1122 ODEs with 24388 terms that describe a stiff chemical reaction network.

```
using ReactionNetworkImporters, OrdinaryDiffEq, DiffEqBiological,
      Sundials, Plots, DiffEqDevTools, ODEInterface, ODEInterfaceDiffEq,
      LSODA
gr()
prnbng = loadrxnetwork(BNGNetwork(), "BNGRepressilator",
                       joinpath(pathof(ReactionNetworkImporters),"..","..",
                       "data","bcr","bcr.net"))
```

```
Error: SystemError: opening file "/home/crackauckas/.julia/packages/Reactio
nNetworkImporters/nZg9K/src/ReactionNetworkImporters.jl/../../data/bcr/bcr.
net": Not a directory
```

```
rn = deepcopy(prnbng.rn)
```

```
Error: UndefVarError: prnbng not defined
```

```
addodes!(rn; build_jac=false, build_symfuncs=false, build_paramjac=false)
```

```
Error: UndefVarError: rn not defined
```

```
tf = 100000.0
oprob = ODEProblem(rn, prnbng.u_0, (0.,tf), prnbng.p);
```

```
Error: UndefVarError: prnbng not defined
```

```
sparsejac_rn = deepcopy(prnbng.rn)
```

```
Error: UndefVarError: prnbng not defined
```

```
addodes!(sparsejac_rn; build_jac=true, sparse_jac = true, build_symfuncs=false,
    build_paramjac=false)
```

```
Error: UndefVarError: sparsejac_rn not defined
```

```
tf = 100000.0
sparsejacprob = ODEProblem(sparsejac_rn, prnbng.u_0, (0.,tf), prnbng.p);
```

```
Error: UndefVarError: prnbng not defined
```

```
@show numspecies(rn) # Number of ODEs
```

```
Error: UndefVarError: rn not defined
```

```
@show numreactions(rn) # Apprx.  number of terms in the ODE
```

```
Error: UndefVarError: rn not defined
```

```
@show numparams(rn) # Number of Parameters
```

```
Error: UndefVarError: rn not defined
```

0.1 Picture of the solution

```
sol = solve(oprob, CVODE_BDF(), saveat=tf/10000., reltol=1e-5, abstol=1e-5)
```

```
Error: UndefVarError: oprob not defined
```

```
plot(sol,legend=false)
```

```
Error: UndefVarError: sol not defined
```

For these benchmarks we will be using the timeseries error with these saving points since the final time point is not well-indicative of the solution behavior (capturing the oscillation is the key!).

0.2 Generate Test Solution

```
@time sol = solve(oprob,CVODE_BDF(),abstol=1/10^12,reltol=1/10^12)
```

```
Error: UndefVarError: oprob not defined
```

```
test_sol = TestSolution(sol)
```

```
Error: UndefVarError: sol not defined
```

0.3 Dense + Automatic Jacobian Solves

Due to the computational cost of the problem, we are only going to focus on the methods which demonstrated computational efficiency on the smaller biochemical benchmark problems. This excludes the exponential integrator, stabilized explicit, and extrapolation classes of methods.

```
abstols = 1.0 ./ 10.0 .^ (5:8)
reltols = 1.0 ./ 10.0 .^ (5:8);
setups = [Dict(:alg=>Rosenbrock23()),
          Dict(:alg=>TRBDF2()),
          Dict(:alg=>CVODE_BDF()),
          Dict(:alg=>rodas()),
          Dict(:alg=>radau()),
          Dict(:alg=>Rodas4()),
          Dict(:alg=>Rodas5()),
          Dict(:alg=>KenCarp4()),
          Dict(:alg=>RadauIIA5()),
          Dict(:alg=>ROS34PW1a()),
          Dict(:alg=>lsoda()),
          ]
wp = WorkPrecisionSet(prob,abstols,reltols,setups;error_estimate=:l2,
                      saveat=tf/10000.,appxsol=test_sol,maxiters=Int(1e5),numruns=1)
```

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

```
plot(wp)
```

```
Error: UndefVarError: wp not defined
```

0.4 Sparse + Analytical Jacobian

```
abstols = 1.0 ./ 10.0 .^ (5:8)
reltols = 1.0 ./ 10.0 .^ (5:8);
setups = [Dict(:alg=>Rosenbrock23()),
          Dict(:alg=>TRBDF2()),
          Dict(:alg=>CVODE_BDF()),
          Dict(:alg=>rodas()),
          Dict(:alg=>radau()),
          Dict(:alg=>Rodas4()),
          Dict(:alg=>Rodas5()),
          Dict(:alg=>KenCarp4()),
          Dict(:alg=>RadauIIA5()),
          Dict(:alg=>ROS34PW1a()),
          Dict(:alg=>lsoda()),
          ]
wp = WorkPrecisionSet(sparsejacprob,abstols,reltols,setups;error_estimate=:l2,
                      saveat=tf/10000.,appxsol=test_sol,maxiters=Int(1e5),numruns=1)
```

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

```
plot(wp)
```

```
Error: UndefVarError: wp not defined
```