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, TimerOutputs

gr()
prnbng = loadrxnetwork(BNGNetwork(), "BNGRepressilator",

joinpath(dirname(pathof(ReactionNetworkImporters)),"..","data","bcr","bcr.net"))
```

```
Parsing parameters...done
Adding parameters...done
Parsing species...done
Adding species...done
Parsing and adding reactions...done
Parsing groups...done
```

```
rn = deepcopy(prnbng.rn)
addodes!(rn; build_jac=false, build_symfuncs=false, build_paramjac=false)
tf = 100000.0
oprob = ODEProblem(rn, prnbng.u_0, (0.,tf), prnbng.p);

densejac_rn = deepcopy(prnbng.rn)
# zeroout_jac=true is needed to keep the generated expressions from being too big for
the compiler
addodes!(densejac_rn; build_jac=true, zeroout_jac = true, sparse_jac = false,
build_symfuncs=false, build_paramjac=false)
densejacprob = ODEProblem(densejac_rn, prnbng.u_0, (0.,tf), prnbng.p);

sparsejac_rn = deepcopy(prnbng.rn)
addodes!(sparsejac_rn; build_jac=true, sparse_jac = true, build_symfuncs=false,
build_paramjac=false)
sparsejacprob = ODEProblem(sparsejac_rn, prnbng.u_0, (0.,tf), prnbng.p);
```

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

```
numspecies(rn) = 1122
```

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

```
numreactions(rn) = 24388
```

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

```
numparams(rn) = 128
128
```

0.1 Time ODE derivative function compilation

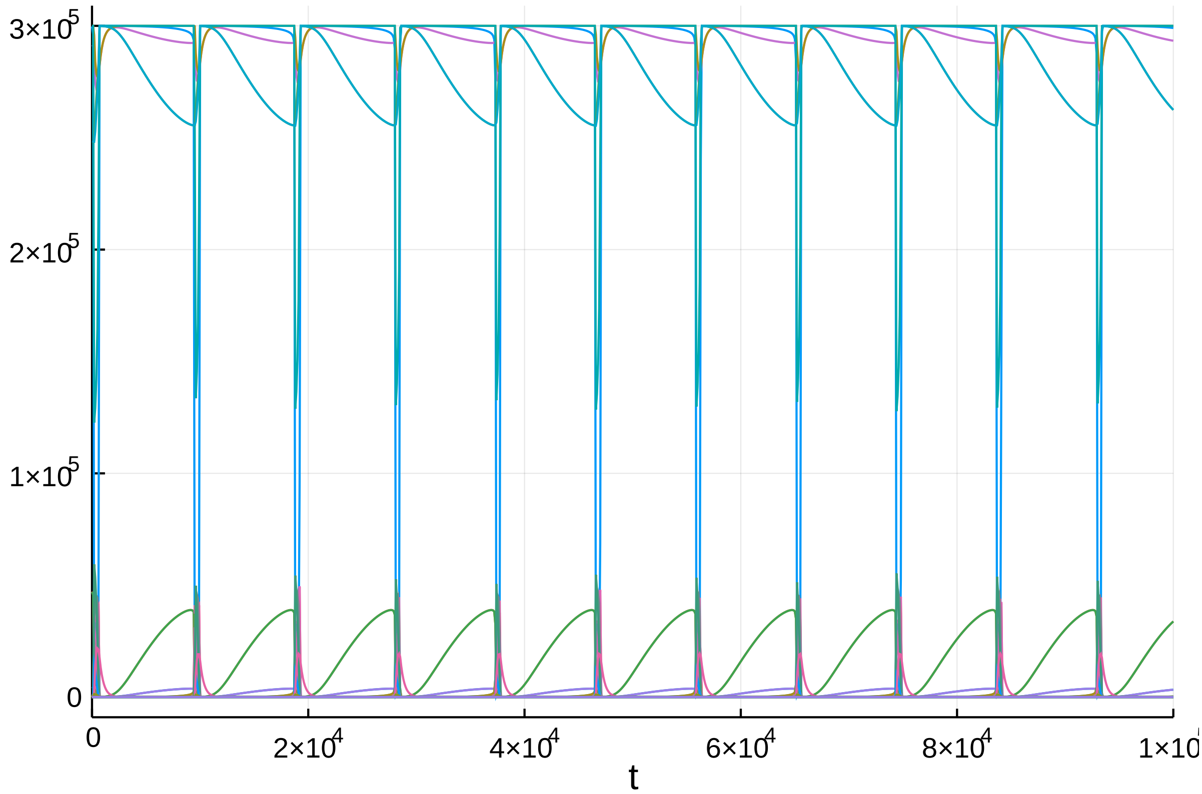
As compiling the ODE derivative functions has in the past taken longer than running a simulation, we first force compilation by evaluating these functions one time.

```
const to = TimerOutput()
u_0 = prnbng.u_0
u = copy(u_0);
du = similar(u);
p = prnbng.p
@timeit to "ODERHS Eval1" rn.f(du,u,p,0.)
@timeit to "ODERHS Eval2" rn.f(du,u,p,0.)
sparsejac_rn.f(du,u,p,0.)

J = zeros(length(u),length(u))
@timeit to "DenseJac Eval1" densejac_rn.jac(J,u,p,0.)
@timeit to "DenseJac Eval2" densejac_rn.jac(J,u,p,0.)

Js = similar(sparsejac_rn.odefun.jac_prototype)
@timeit to "SparseJac Eval1" sparsejac_rn.jac(Js,u,p,0.)
@timeit to "SparseJac Eval2" sparsejac_rn.jac(Js,u,p,0.)
show(to)
```

```
                                    Time                    Allocations

     Tot / % measured:          156s / 85.5%           17.1GiB / 80.6%

 Section              ncalls     time    %tot     avg     alloc    %tot      avg

 DenseJac Eval1            1    64.6s   48.6%   64.6s   5.27GiB   38.3%  5.27GiB
 SparseJac Eval1           1    46.0s   34.6%   46.0s   5.21GiB   37.8%  5.21GiB
 ODERHS Eval1              1    22.4s   16.9%   22.4s   3.30GiB   23.9%  3.30GiB
 DenseJac Eval2            1    572μs   0.00%   572μs     32.0B   0.00%    32.0B
 SparseJac Eval2           1   50.7μs   0.00%  50.7μs     32.0B   0.00%    32.0B
 ODERHS Eval2              1   39.2μs   0.00%  39.2μs     32.0B   0.00%    32.0B
```

0.2 Picture of the solution

```
sol = solve(oprob, CVODE_BDF(), saveat=tf/1000., reltol=1e-5, abstol=1e-5)
plot(sol,legend=false, fmt=:png)
```



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!).

0.3 Generate Test Solution

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

```
598.747572 seconds (5.55 M allocations: 2.225 GiB, 0.28% gc time)
```

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

```
retcode: Success
Interpolation: 3rd order Hermite
t: nothing
u: nothing
```

0.4 Setups

```
abstols = 1.0 ./ 10.0 .^ (5:8)
reltols = 1.0 ./ 10.0 .^ (5:8);
setups = [
          #Dict(:alg=>Rosenbrock23(autodiff=false)),
          Dict(:alg=>TRBDF2(autodiff=false)),
          Dict(:alg=>CVODE_BDF()),
          #Dict(:alg=>rodas()),
          #Dict(:alg=>radau()),
          #Dict(:alg=>Rodas4(autodiff=false)),
          #Dict(:alg=>Rodas5(autodiff=false)),
          Dict(:alg=>KenCarp4(autodiff=false)),
          #Dict(:alg=>RadauIIA5(autodiff=false)),
          #Dict(:alg=>lsoda()),
```

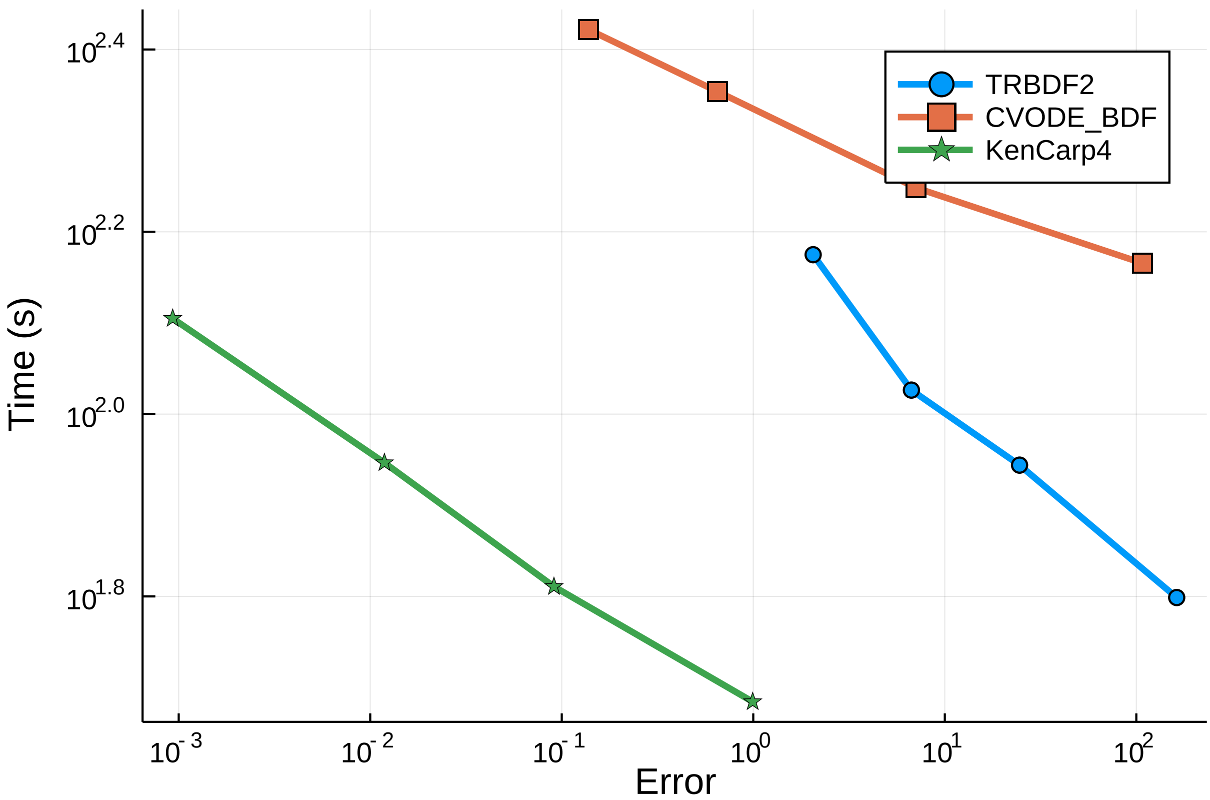
```
        ]

3-element Array{Dict{Symbol,V} where V,1}:
 Dict(:alg => OrdinaryDiffEq.TRBDF2{0,false,DiffEqBase.DefaultLinSolve,Diff
EqBase.NLNewton{Rational{Int64},Rational{Int64},Rational{Int64}},DataType}(
DiffEqBase.DefaultLinSolve(nothing, nothing), DiffEqBase.NLNewton{Rational{
Int64},Rational{Int64},Rational{Int64}}(1//100, 10, 1//5, 1//5), Val{:forwa
rd}, true, :linear, :PI))
 Dict(:alg => Sundials.CVODE_BDF{:Newton,:Dense,Nothing,Nothing}(0, 0, 0, 0
, false, 10, 5, 7, 3, 10, nothing, nothing, 0))


 Dict(:alg => OrdinaryDiffEq.KenCarp4{0,false,DiffEqBase.DefaultLinSolve,Di
ffEqBase.NLNewton{Rational{Int64},Rational{Int64},Rational{Int64}},DataType
}(DiffEqBase.DefaultLinSolve(nothing, nothing), DiffEqBase.NLNewton{Rationa
l{Int64},Rational{Int64},Rational{Int64}}(1//100, 10, 1//5, 1//5), Val{:for
ward}, true, :linear, :PI))
```

0.5 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.

First we test using auto-generated Jacobians (finite difference)

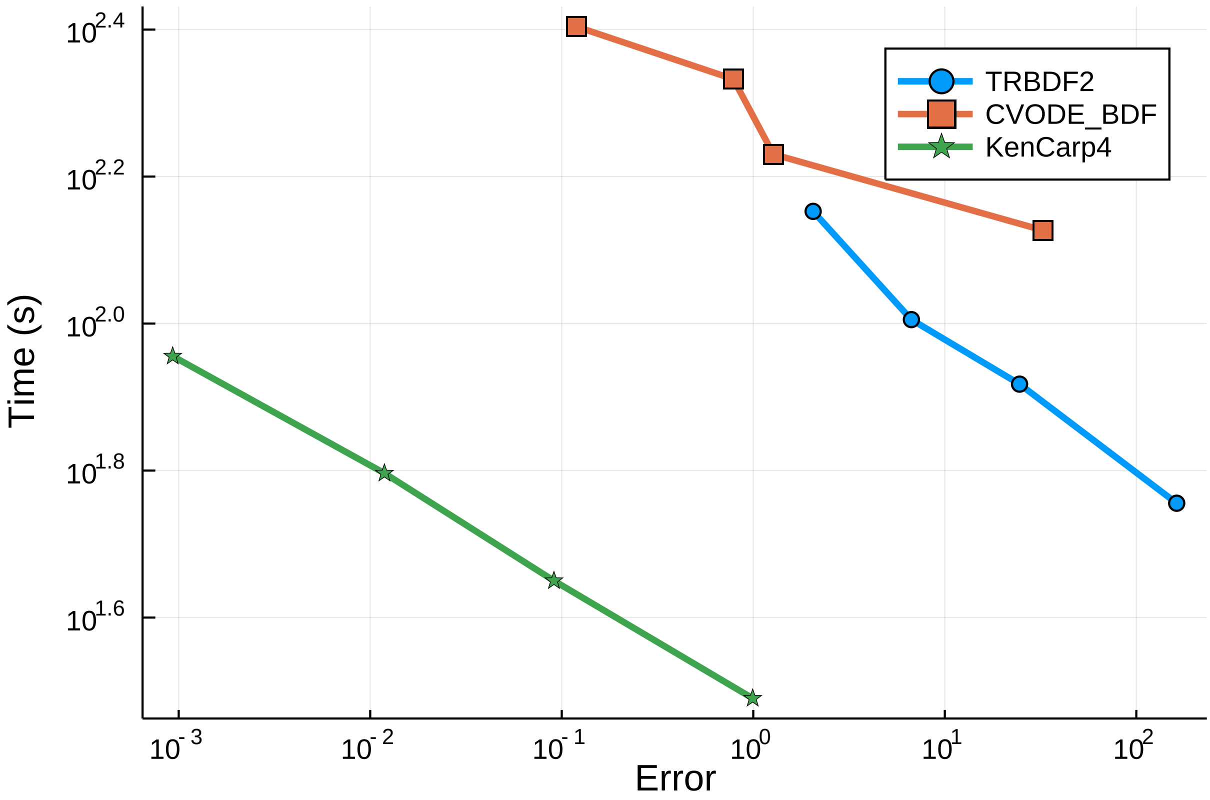
```
wp = WorkPrecisionSet(oprob,abstols,reltols,setups;error_estimate=:l2,
                      saveat=tf/10000.,appxsol=test_sol,maxiters=Int(1e5),numruns=1)
plot(wp)
```



0.6 Analytical Jacobian

Now we test using the generated analytic Jacobian function.

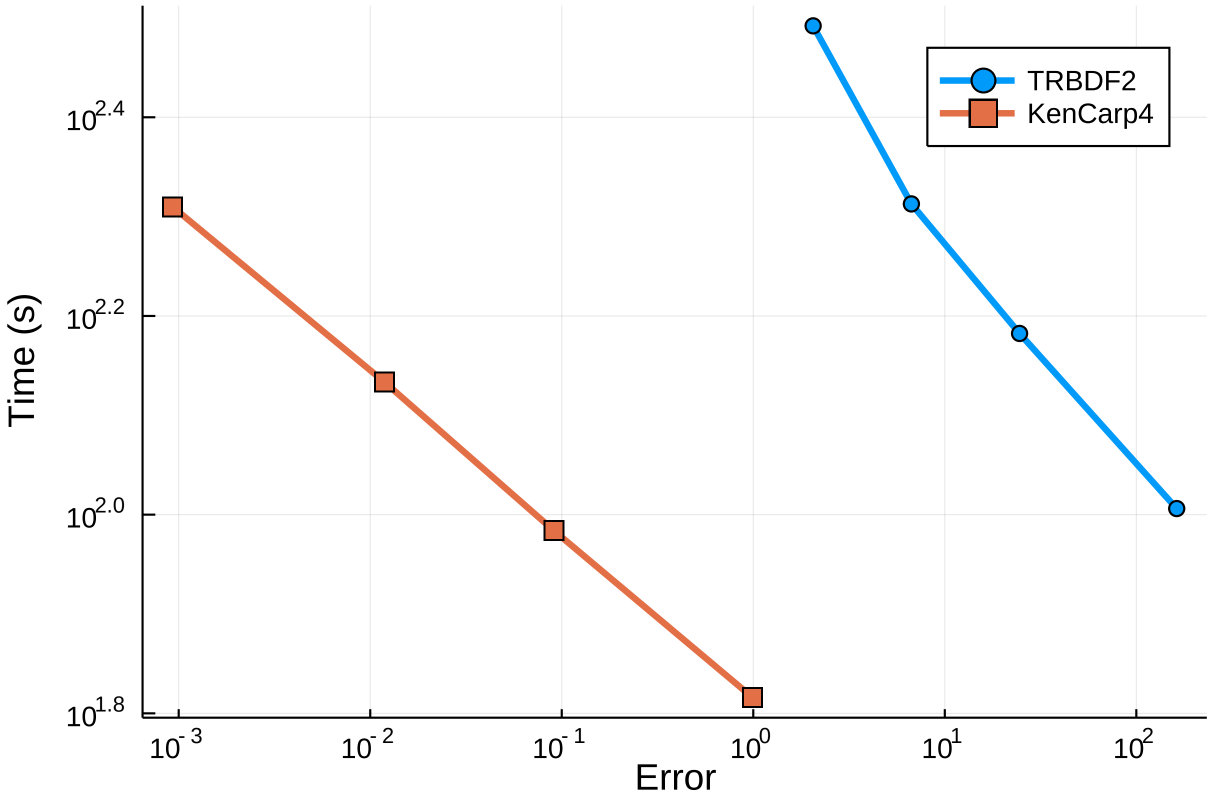
```
wp = WorkPrecisionSet(densejacprob,abstols,reltols,setups;error_estimate=:l2,
                      saveat=tf/10000.,appxsol=test_sol,maxiters=Int(1e5),numruns=1)
plot(wp)
```



0.7 Sparse Jacobian

Finally we test using the generated sparse analytic Jacobian function.

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



TRBDF2
KenCarp4
Time (s)
$10^{2.4}$
$10^{2.2}$
$10^{2.0}$
$10^{1.8}$
10^{-3}
10^{-2}
10^{-1}
10^{0}
10^{1}
10^{2}
Error