

Filament Work-Precision Diagrams

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August 2, 2019

1 Filament Benchmark

In this notebook we will benchmark a real-world biological model from a paper entitled [Magnetic dipole with a flexible tail as a self-propelling microdevice](#). This is a system of PDEs representing a Kirchhoff model of an elastic rod, where the equations of motion are given by the Rouse approximation with free boundary conditions.

1.1 Model Implementation

First we will show the full model implementation. It is not necessary to understand the full model specification in order to understand the benchmark results, but it's all contained here for completeness. The model is highly optimized, with all internal vectors pre-cached, loops unrolled for efficiency (along with `@simd` annotations), a pre-defined Jacobian, matrix multiplications are all in-place, etc. Thus this model is a good stand-in for other optimized PDE solving cases.

The model is thus defined as follows:

```
using OrdinaryDiffEq, ODEInterfaceDiffEq, Sundials, DiffEqDevTools, LSODA
using LinearAlgebra
using Plots
gr()

Plots.GRBackend()

const T = Float64
abstract type AbstractFilamentCache end
abstract type AbstractMagneticForce end
abstract type AbstractInextensibilityCache end
abstract type AbstractSolver end
abstract type AbstractSolverCache end

struct FerromagneticContinuous <: AbstractMagneticForce
    ω :: T
    F :: Vector{T}
end

mutable struct FilamentCache{
    MagneticForce <: AbstractMagneticForce,
    InextensibilityCache <: AbstractInextensibilityCache,
    SolverCache <: AbstractSolverCache
```

```

        } <: AbstractFilamentCache
N :: Int
μ :: T
Cm :: T
x :: SubArray{T,1,Vector{T},Tuple{StepRange{Int,Int}},true}
y :: SubArray{T,1,Vector{T},Tuple{StepRange{Int,Int}},true}
z :: SubArray{T,1,Vector{T},Tuple{StepRange{Int,Int}},true}
A :: Matrix{T}
P :: InextensibilityCache
F :: MagneticForce
Sc :: SolverCache
end

struct NoHydroProjectionCache <: AbstractInextensibilityCache
    J      :: Matrix{T}
    P      :: Matrix{T}
    J_JT   :: Matrix{T}
    J_JT_LDLT :: LinearAlgebra.LDLt{T, SymTridiagonal{T}}
    P0     :: Matrix{T}

    NoHydroProjectionCache(N::Int) = new(
        zeros(N, 3*(N+1)),      # J
        zeros(3*(N+1), 3*(N+1)), # P
        zeros(N,N),             # J_JT
        LinearAlgebra.LDLt{T,SymTridiagonal{T}}(SymTridiagonal(zeros(N), zeros(N-1))),
        zeros(N, 3*(N+1))
    )
end

struct DiffEqSolverCache <: AbstractSolverCache
    S1 :: Vector{T}
    S2 :: Vector{T}

    DiffEqSolverCache(N::Integer) = new(zeros(T,3*(N+1)), zeros(T,3*(N+1)))
end

function FilamentCache(N=20; Cm=32, ω=200, Solver=SolverDiffEq)
    InextensibilityCache = NoHydroProjectionCache
    SolverCache = DiffEqSolverCache
    tmp = zeros(3*(N+1))
    FilamentCache{FerromagneticContinuous, InextensibilityCache, SolverCache}(
        N, N+1, Cm, view(tmp,1:3:3*(N+1)), view(tmp,2:3:3*(N+1)), view(tmp,3:3:3*(N+1)),
        zeros(3*(N+1), 3*(N+1)), # A
        InextensibilityCache(N), # P
        FerromagneticContinuous(ω, zeros(3*(N+1))),
        SolverCache(N)
    )
end

Main.WeaveSandBox1.FilamentCache

function stiffness_matrix!(f::AbstractFilamentCache)
    N, μ, A = f.N, f.μ, f.A
    @inbounds for j in axes(A, 2), i in axes(A, 1)
        A[i, j] = j == i ? 1 : 0
    end
    @inbounds for i in 1 : 3
        A[i,i] = 1
        A[i,3+i] = -2
        A[i,6+i] = 1
    end
end

```

```

A[3+i,i] = -2
A[3+i,3+i] = 5
A[3+i,6+i] = -4
A[3+i,9+i] = 1

A[3*(N-1)+i,3*(N-3)+i] = 1
A[3*(N-1)+i,3*(N-2)+i] = -4
A[3*(N-1)+i,3*(N-1)+i] = 5
A[3*(N-1)+i,3*N+i] = -2

A[3*N+i,3*(N-2)+i] = 1
A[3*N+i,3*(N-1)+i] = -2
A[3*N+i,3*N+i] = 1

for j in 2 : N-2
    A[3*j+i,3*j+i] = 6
    A[3*j+i,3*(j-1)+i] = -4
    A[3*j+i,3*(j+1)+i] = -4
    A[3*j+i,3*(j-2)+i] = 1
    A[3*j+i,3*(j+2)+i] = 1
end
end
rmul!(A, -μ^4)
nothing
end

stiffness_matrix! (generic function with 1 method)

function update_separate_coordinates!(f::AbstractFilamentCache, r)
    N, x, y, z = f.N, f.x, f.y, f.z
    @inbounds for i in 1 : length(x)
        x[i] = r[3*i-2]
        y[i] = r[3*i-1]
        z[i] = r[3*i]
    end
    nothing
end

function update_united_coordinates!(f::AbstractFilamentCache, r)
    N, x, y, z = f.N, f.x, f.y, f.z
    @inbounds for i in 1 : length(x)
        r[3*i-2] = x[i]
        r[3*i-1] = y[i]
        r[3*i] = z[i]
    end
    nothing
end

function update_united_coordinates(f::AbstractFilamentCache)
    r = zeros(T, 3*length(f.x))
    update_united_coordinates!(f, r)
    r
end

update_united_coordinates (generic function with 1 method)

function initialize!(initial_conf_type::Symbol, f::AbstractFilamentCache)
    N, x, y, z = f.N, f.x, f.y, f.z
    if initial_conf_type == :StraightX

```

```

        x .= range(0, stop=1, length=N+1)
        y .= 0
        z .= 0
    else
        error("Unknown initial configuration requested.")
    end
    update_united_coordinates(f)
end

initialize! (generic function with 1 method)

function magnetic_force! (::FerromagneticContinuous, f::AbstractFilamentCache, t)
    # TODO: generalize this for different magnetic fields as well
    N,  $\mu$ , Cm,  $\omega$ , F = f.N, f. $\mu$ , f.Cm, f.F. $\omega$ , f.F.F
    F[1] = - $\mu$  * Cm * cos( $\omega$ *t)
    F[2] = - $\mu$  * Cm * sin( $\omega$ *t)
    F[3*(N+1)-2] =  $\mu$  * Cm * cos( $\omega$ *t)
    F[3*(N+1)-1] =  $\mu$  * Cm * sin( $\omega$ *t)
    nothing
end

magnetic_force! (generic function with 1 method)

struct SolverDiffEq <: AbstractSolver end

function (f::FilamentCache)(dr, r, p, t)
    @views f.x, f.y, f.z = r[1:3:end], r[2:3:end], r[3:3:end]
    jacobian!(f)
    projection!(f)
    magnetic_force!(f.F, f, t)
    A, P, F, S1, S2 = f.A, f.P.P, f.F.F, f.Sc.S1, f.Sc.S2

    # implement dr = P * (A*r + F) in an optimized way to avoid temporaries
    mul!(S1, A, r)
    S1 .+= F
    mul!(S2, P, S1)
    copyto!(dr, S2)
    return dr
end

function jacobian!(f::FilamentCache)
    N, x, y, z, J = f.N, f.x, f.y, f.z, f.P.J
    @inbounds for i in 1 : N
        J[i, 3*i-2] = -2 * (x[i+1]-x[i])
        J[i, 3*i-1] = -2 * (y[i+1]-y[i])
        J[i, 3*i] = -2 * (z[i+1]-z[i])
        J[i, 3*(i+1)-2] = 2 * (x[i+1]-x[i])
        J[i, 3*(i+1)-1] = 2 * (y[i+1]-y[i])
        J[i, 3*(i+1)] = 2 * (z[i+1]-z[i])
    end
    nothing
end

jacobian! (generic function with 1 method)

function projection!(f::FilamentCache)
    # implement P[:, :] = I - J'/(J*J')*J in an optimized way to avoid temporaries
    J, P, J_JT, J_JT_LDLT, P0 = f.P.J, f.P.P, f.P.J_JT, f.P.J_JT_LDLT, f.P.P0
    mul!(J_JT, J, J')
    LDLt_inplace!(J_JT_LDLT, J_JT)

```

```

    ldiv!(P0, J_JT_LDLT, J)
    mul!(P, P0', J)
    subtract_from_identity!(P)
    nothing
end

projection! (generic function with 1 method)

function subtract_from_identity!(A)
    lmul!(-1, A)
    @inbounds for i in 1 : size(A,1)
        A[i,i] += 1
    end
    nothing
end

subtract_from_identity! (generic function with 1 method)

function LDLt_inplace!(L::LinearAlgebra.LDLt{T,SymTridiagonal{T}}, A::Matrix{T}) where
    {T<:Real}
    n = size(A,1)
    dv, ev = L.data.dv, L.data.ev
    @inbounds for (i,d) in enumerate(diagind(A))
        dv[i] = A[d]
    end
    @inbounds for (i,d) in enumerate(diagind(A,-1))
        ev[i] = A[d]
    end
    @inbounds @simd for i in 1 : n-1
        ev[i] /= dv[i]
        dv[i+1] -= abs2(ev[i]) * dv[i]
    end
    L
end

LDLt_inplace! (generic function with 1 method)

```

2 Investigating the model

Let's take a look at what results of the model look like:

```

function run(::SolverDiffEq; N=20, Cm=32, ω=200, time_end=1.,
    solver=TRBDF2(autodiff=false), reltol=1e-6, abstol=1e-6)
    f = FilamentCache(N, Solver=SolverDiffEq, Cm=Cm, ω=ω)
    r0 = initialize!(StraightX, f)
    stiffness_matrix!(f)
    prob = ODEProblem(ODEFunction(f, jac=(J, u, p, t)->(mul!(J, f.P.P, f.A); nothing)),
        r0, (0., time_end))
    sol = solve(prob, solver, dense=false, reltol=reltol, abstol=abstol)
end

run (generic function with 1 method)

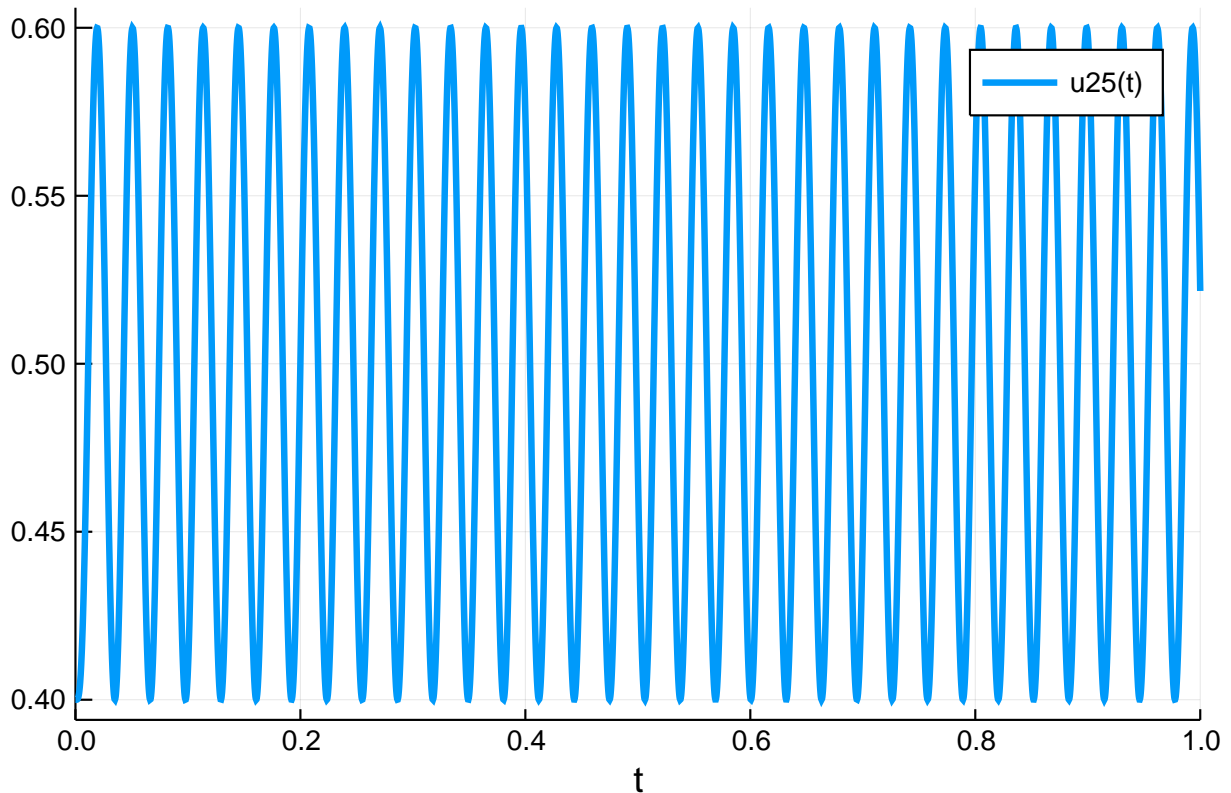
```

This method runs the model with the TRBDF2 method and the default parameters.

```

sol = run(SolverDiffEq())
plot(sol, vars = (0,25))

```



The model quickly falls into a highly oscillatory mode which then dominates throughout the rest of the solution.

3 Work-Precision Diagrams

Now let's build the problem and solve it once at high accuracy to get a reference solution:

```
N=20
f = FilamentCache(N, Solver=SolverDiffEq)
r0 = initialize!(StraightX, f)
stiffness_matrix!(f)
prob = ODEProblem(f, r0, (0., 0.01))

sol = solve(prob, Vern9(), reltol=1e-14, abstol=1e-14)
test_sol = TestSolution(sol);
```

3.1 High Tolerance (Low Accuracy)

3.1.1 Endpoint Error

ODEInterfaceDiffEq solvers failed to run.

```
abstols=1 ./10 .^(3:8)
reltols=1 ./10 .^(3:8)
setups = [
    Dict(:alg => CVODE_BDF()),
    Dict(:alg => Rosenbrock23(autodiff=false)),
    Dict(:alg => Rodas4(autodiff=false)),
```

```

Dict(:alg => BS3()),
Dict(:alg => Tsit5()),
Dict(:alg => ImplicitEuler(autodiff=false)),
Dict(:alg => Trapezoid(autodiff=false)),
Dict(:alg => TRBDF2(autodiff=false)),
Dict(:alg => radau()),
Dict(:alg => rodas()),
Dict(:alg => dop853()),
#Dict(:alg => lsoda())
];

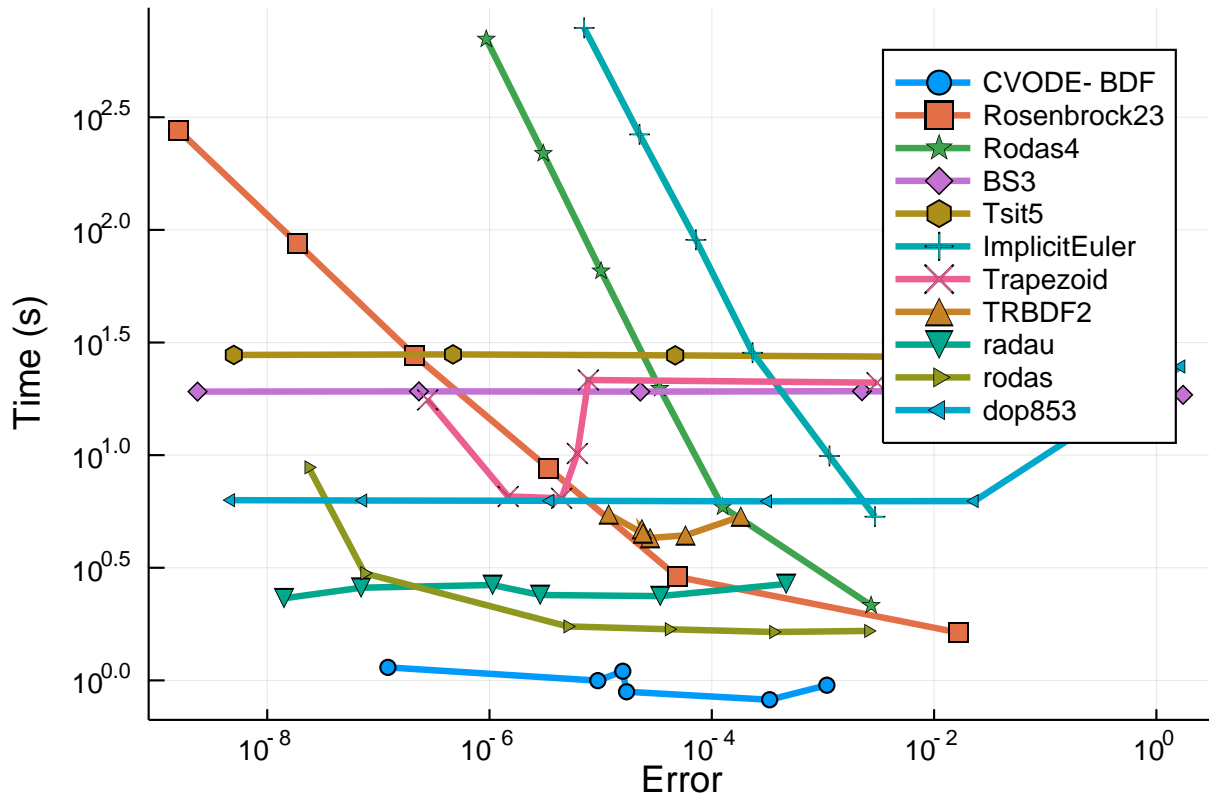
names = [
  "CVODE-BDF",
  "Rosenbrock23",
  "Rodas4",
  "BS3",
  "Tsit5",
  "ImplicitEuler",
  "Trapezoid",
  "TRBDF2",
  "radau",
  "rodas",
  "dop853",
  #"lsoda"
];

wp = WorkPrecisionSet(prob, abstols, reltols, setups; names=names, appxsol=test_sol,
  maxiters=Int(1e6), verbose = false)

EXIT OF RADAU AT X=          0.1000E-01
STEP SIZE TOO SMALL, H=    1.7347234759768071E-018
EXIT OF RADAU AT X=          0.1000E-01
STEP SIZE TOO SMALL, H=    1.7347234759768071E-018
EXIT OF RADAU AT X=          0.1000E-01
STEP SIZE TOO SMALL, H=    1.7347234759768071E-018

plot(wp)

```



```

abstols=1 ./10 .^(3:8)
reltols=1 ./10 .^(3:8)
setups = [
    Dict(:alg => CVODE_BDF()),
    Dict(:alg => Rosenbrock23(autodiff=false)),
    Dict(:alg => Rodas4(autodiff=false)),
    Dict(:alg => ImplicitEuler(autodiff=false)),
    Dict(:alg => TRBDF2(autodiff=false)),
    Dict(:alg => radau()),
    Dict(:alg => KenCarp3(autodiff=false)),
    Dict(:alg => KenCarp4(autodiff=false)),
    Dict(:alg => Kvaerno3(autodiff=false)),
    Dict(:alg => Kvaerno4(autodiff=false)),
    Dict(:alg => ROCK2()),
    Dict(:alg => ROCK4())
];

```

```

names = [
    "CVODE-BDF",
    "Rosenbrock23",
    "Rodas4",
    "ImplicitEuler",
    "TRBDF2",
    "radau",
    "KenCarp3",
    "KenCarp4",
    "Kvaerno3",
    "Kvaerno4",
    "ROCK2",
    "ROCK4"
];

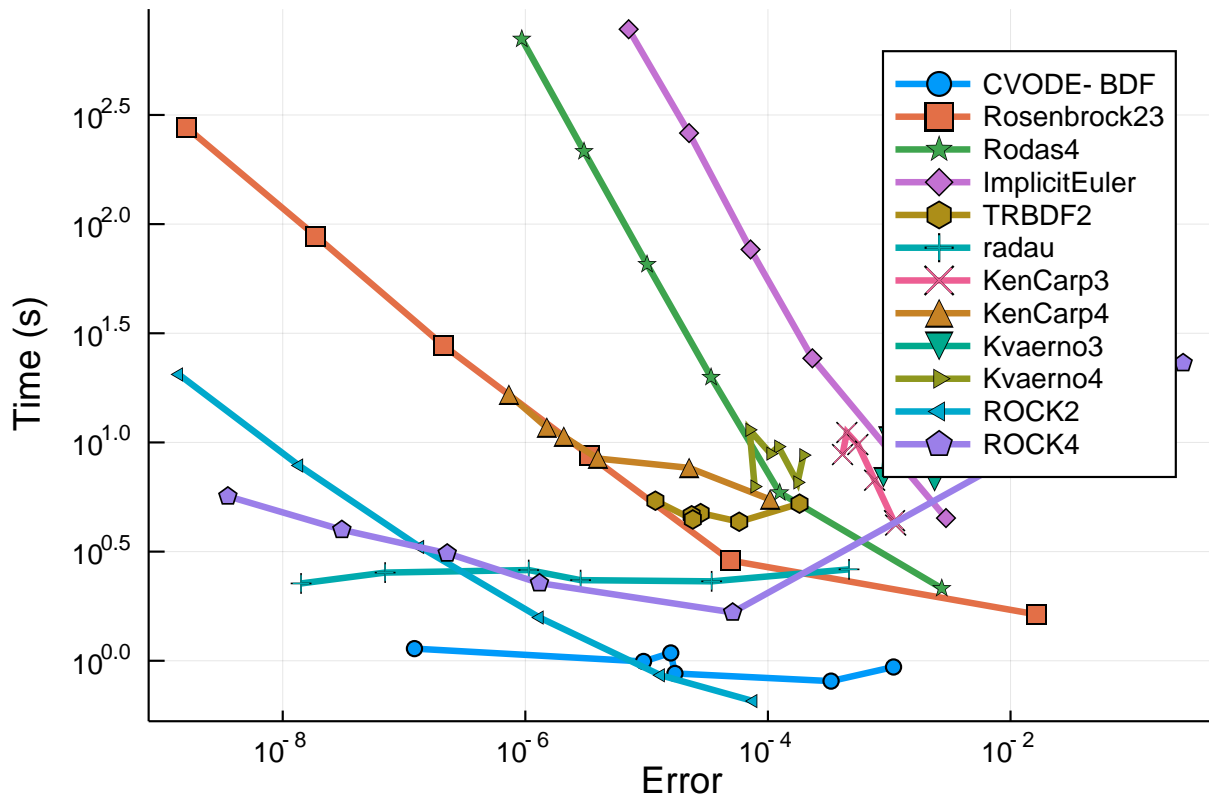
```



```
wp = WorkPrecisionSet(prob, abstols, reltols, setups; names=names, appxsol=test_sol,
    maxiters=Int(1e6), verbose = false)
```

```
EXIT OF RADAU AT X=      0.1000E-01
STEP SIZE TOO SMALL, H= 1.7347234759768071E-018
EXIT OF RADAU AT X=      0.1000E-01
STEP SIZE TOO SMALL, H= 1.7347234759768071E-018
EXIT OF RADAU AT X=      0.1000E-01
STEP SIZE TOO SMALL, H= 1.7347234759768071E-018
```

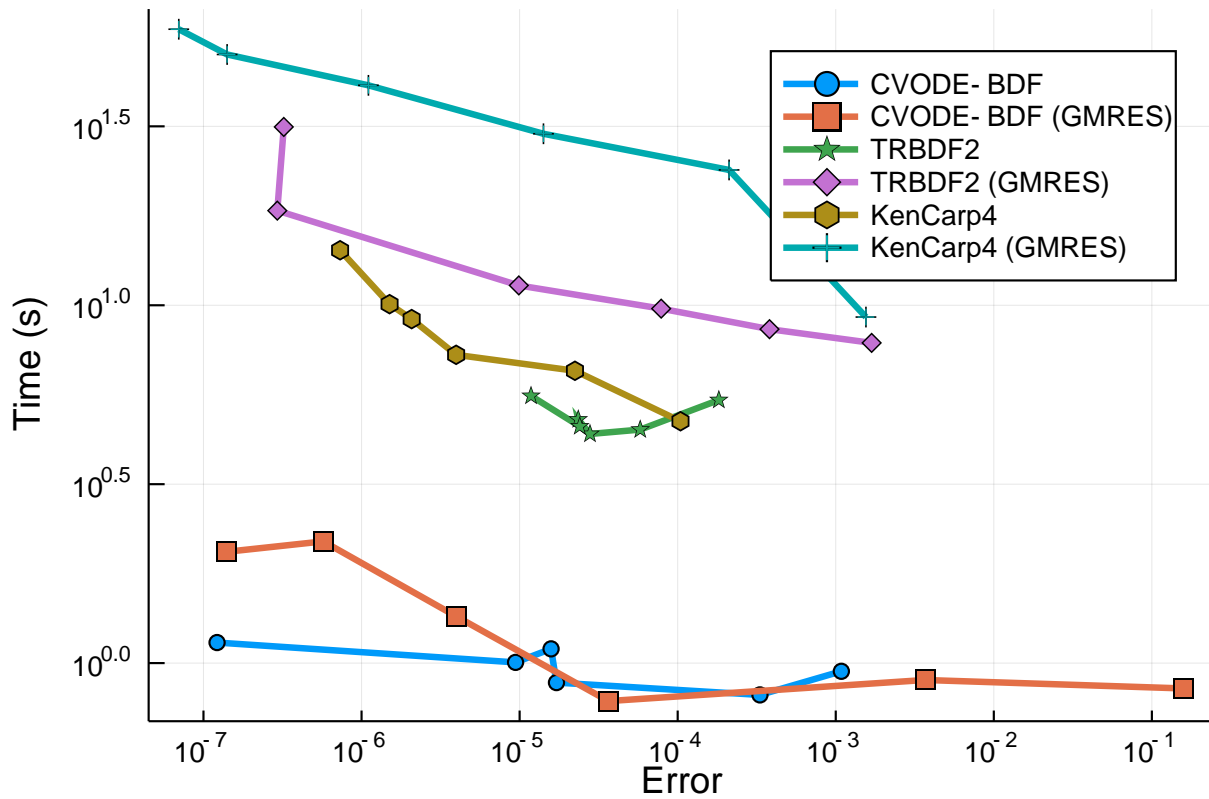
```
plot(wp)
```



```
abstols=1 ./10 .^(3:8)
reltols=1 ./10 .^(3:8)
setups = [
    Dict(:alg => CVODE_BDF()),
    Dict(:alg => CVODE_BDF(linear_solver=:GMRES)),
    Dict(:alg => TRBDF2(autodiff=false)),
    Dict(:alg => TRBDF2(autodiff=false,linsolve=LinSolveGMRES())),
    Dict(:alg => KenCarp4(autodiff=false)),
    Dict(:alg => KenCarp4(autodiff=false,linsolve=LinSolveGMRES())),
];

names = [
    "CVODE-BDF",
    "CVODE-BDF (GMRES)",
    "TRBDF2",
    "TRBDF2 (GMRES)",
    "KenCarp4",
    "KenCarp4 (GMRES)",
];
```

```
wp = WorkPrecisionSet(prob, abstols, reltols, setups; names=names, appxsol=test_sol,
    maxiters=Int(1e6), verbose = false)
plot(wp)
```



3.1.2 Timeseries Error

```
abstols=1 ./10 .^(3:8)
reltols=1 ./10 .^(3:8)
setups = [
    Dict(:alg => CVMODE_BDF()),
    Dict(:alg => Rosenbrock23(autodiff=false)),
    Dict(:alg => Rodas4(autodiff=false)),
    Dict(:alg => Trapezoid(autodiff=false)),
    Dict(:alg => TRBDF2(autodiff=false)),
    Dict(:alg => radau()),
    Dict(:alg => rodas()),
    #Dict(:alg => lsoda()),
    Dict(:alg => ROCK2()),
    Dict(:alg => ROCK4())
];

names = [
    "CVMODE-BDF",
    "Rosenbrock23",
    "Rodas4",
    "Trapezoid",
    "TRBDF2",
    "radau",
    "rodas",
    #"lsoda",
    "ROCK2",

```

```

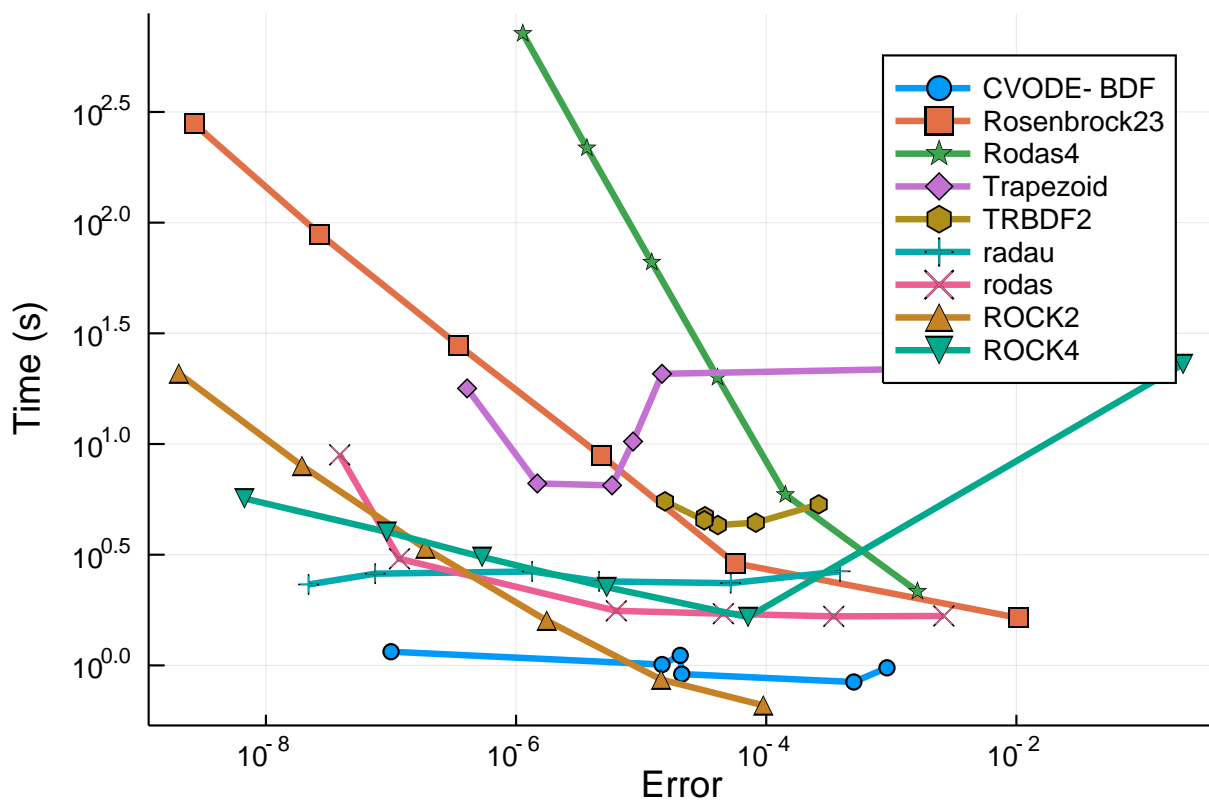
"ROCK4"
];

wp = WorkPrecisionSet(prob, abstols, reltols, setups; names=names, appxsol=test_sol,
    dense = false,
    maxiters=Int(1e6), verbose = false, error_estimate=:l2)

EXIT OF RADAU AT X=      0.1000E-01
STEP SIZE TOO SMALL, H= 1.7347234759768071E-018
EXIT OF RADAU AT X=      0.1000E-01
STEP SIZE TOO SMALL, H= 1.7347234759768071E-018
EXIT OF RADAU AT X=      0.1000E-01
STEP SIZE TOO SMALL, H= 1.7347234759768071E-018

plot(wp)

```



By looking at the previous plots, we can see that TRBDF2 is the quicker one and lsoda is the slower one (the colors are similar!)

```

abstols=1 ./10 .^(3:8)
reltols=1 ./10 .^(3:8)
setups = [
    Dict(:alg => CVODE_BDF()),
    Dict(:alg => Rosenbrock23(autodiff=false)),
    Dict(:alg => Rodas4(autodiff=false)),
    Dict(:alg => TRBDF2(autodiff=false)),
    Dict(:alg => radau()),
    Dict(:alg => KenCarp3(autodiff=false)),
    Dict(:alg => KenCarp4(autodiff=false)),
    Dict(:alg => Kvaerno3(autodiff=false)),
    Dict(:alg => Kvaerno4(autodiff=false)),
    Dict(:alg => ROCK2()),

```

```

Dict(:alg => ROCK4())
];

names = [
    "CVODE-BDF",
    "Rosenbrock23",
    "Rodas4",
    "TRBDF2",
    "radau",
    "KenCarp3",
    "KenCarp4",
    "Kvaerno3",
    "Kvaerno4",
    "ROCK2",
    "ROCK4"
];

wp = WorkPrecisionSet(prob, abstols, reltols, setups; names=names, appxsol=test_sol,
    maxiters=Int(1e6), verbose = false)

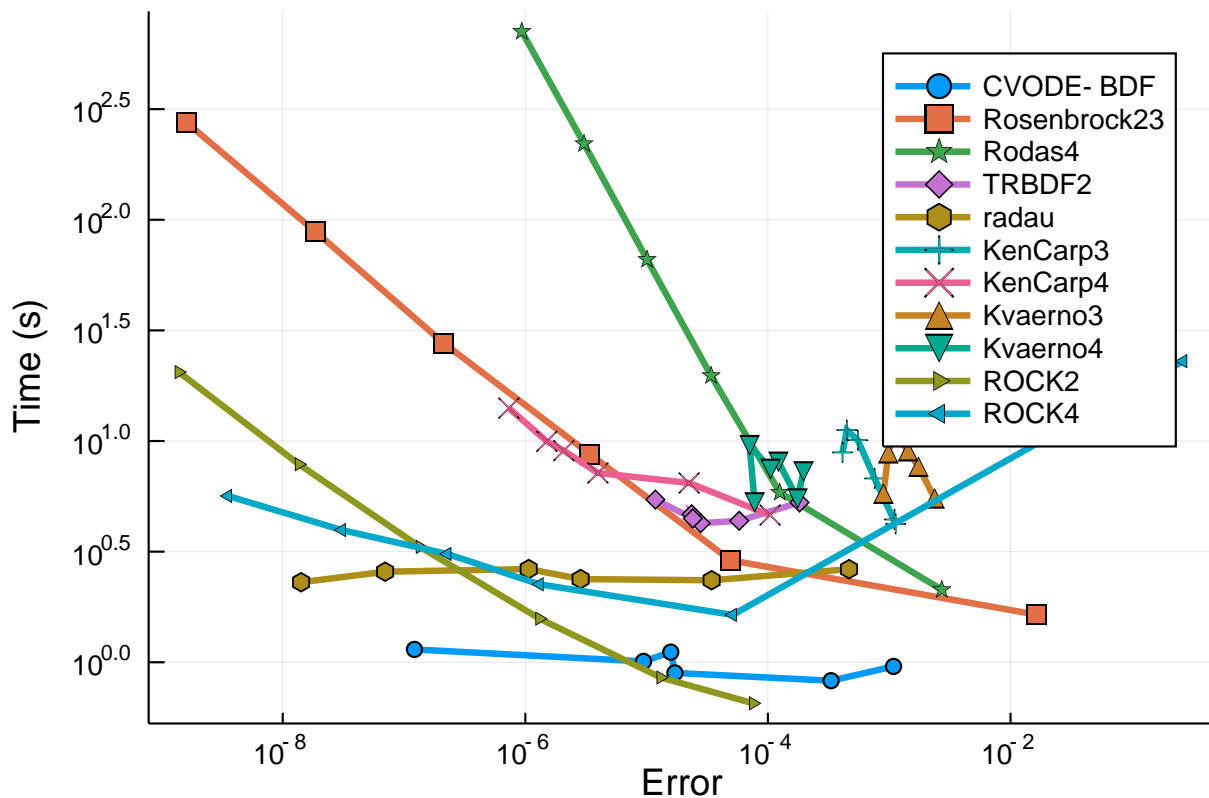
```

```

EXIT OF RADAU AT X=      0.1000E-01
STEP SIZE TOO SMALL, H= 1.7347234759768071E-018
EXIT OF RADAU AT X=      0.1000E-01
STEP SIZE TOO SMALL, H= 1.7347234759768071E-018
EXIT OF RADAU AT X=      0.1000E-01
STEP SIZE TOO SMALL, H= 1.7347234759768071E-018

```

```
plot(wp)
```



3.1.3 Dense Error

```
abstols=1 ./10 .^(3:8)
```

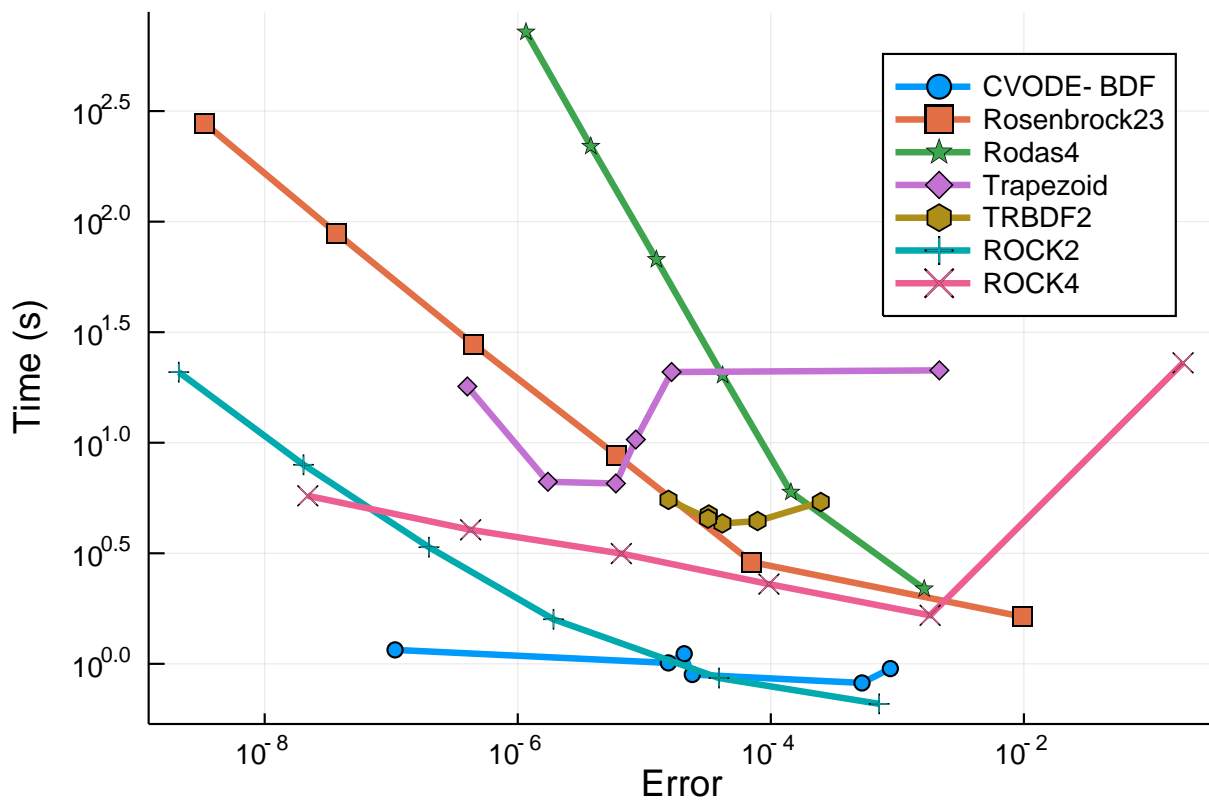
```

reltols=1 ./10 .^(3:8)
setups = [
    Dict(:alg => CVODE_BDF()),
    Dict(:alg => Rosenbrock23(autodiff=false)),
    Dict(:alg => Rodas4(autodiff=false)),
    Dict(:alg => Trapezoid(autodiff=false)),
    Dict(:alg => TRBDF2(autodiff=false)),
    Dict(:alg => ROCK2()),
    Dict(:alg => ROCK4())
];

names = [
    "CVODE-BDF",
    "Rosenbrock23",
    "Rodas4",
    "Trapezoid",
    "TRBDF2",
    "ROCK2",
    "ROCK4"
];

wp = WorkPrecisionSet(prob, abstols, reltols, setups; names=names, appxsol=test_sol,
    dense=true,
    maxiters=Int(1e6), verbose = false, dense_errors = true,
    error_estimate=:L2)
plot(wp)

```



```

abstols=1 ./10 .^(3:8)
reltols=1 ./10 .^(3:8)
setups = [
    Dict(:alg => CVODE_BDF()),
    Dict(:alg => Rosenbrock23(autodiff=false)),

```

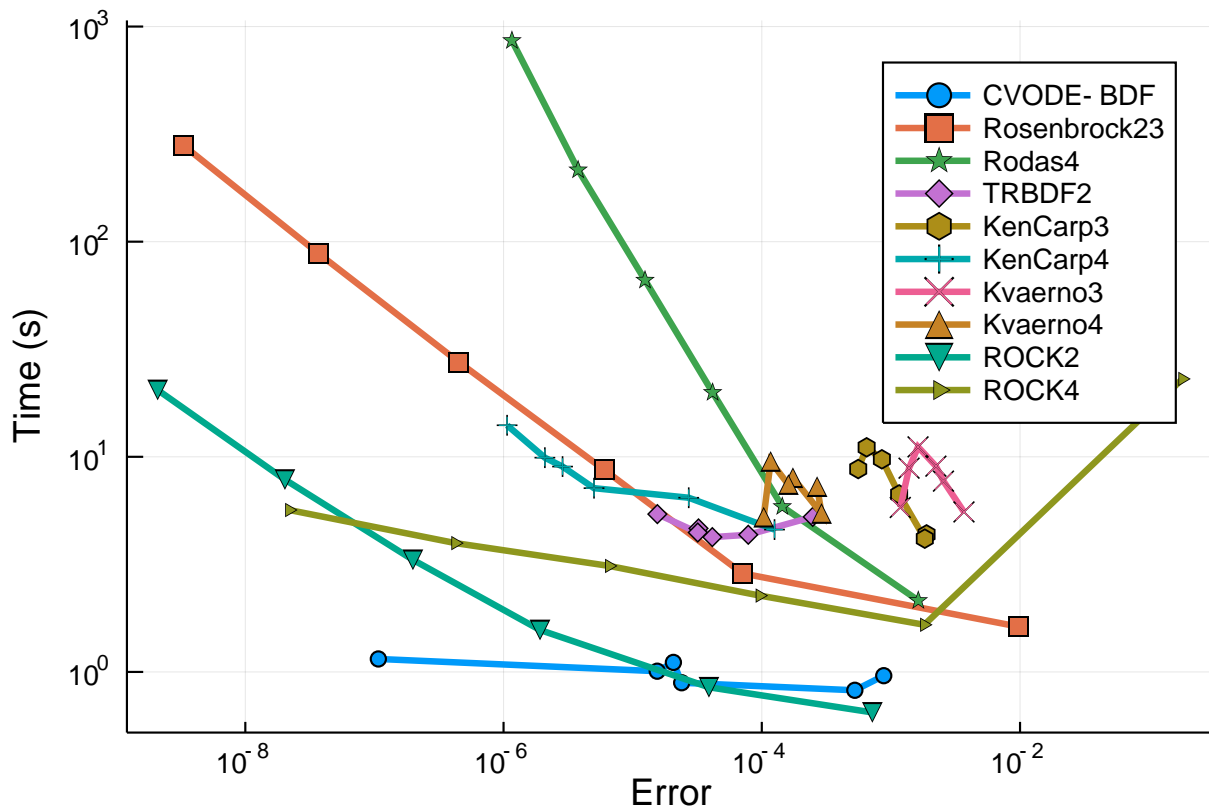
```

Dict(:alg => Rodas4(autodiff=false)),
Dict(:alg => TRBDF2(autodiff=false)),
Dict(:alg => KenCarp3(autodiff=false)),
Dict(:alg => KenCarp4(autodiff=false)),
Dict(:alg => Kvaerno3(autodiff=false)),
Dict(:alg => Kvaerno4(autodiff=false)),
Dict(:alg => ROCK2()),
Dict(:alg => ROCK4())
];

names = [
    "CVODE-BDF",
    "Rosenbrock23",
    "Rodas4",
    "TRBDF2",
    "KenCarp3",
    "KenCarp4",
    "Kvaerno3",
    "Kvaerno4",
    "ROCK2",
    "ROCK4"
];

wp = WorkPrecisionSet(prob, abstols, reltols, setups; names=names, appxsol=test_sol,
    maxiters=Int(1e6), verbose = false, dense_errors = true,
    error_estimate=:L2)
plot(wp)

```



3.2 Low Tolerance (High Accuracy)

```
abstols=1 ./10 .^(6:12)
```

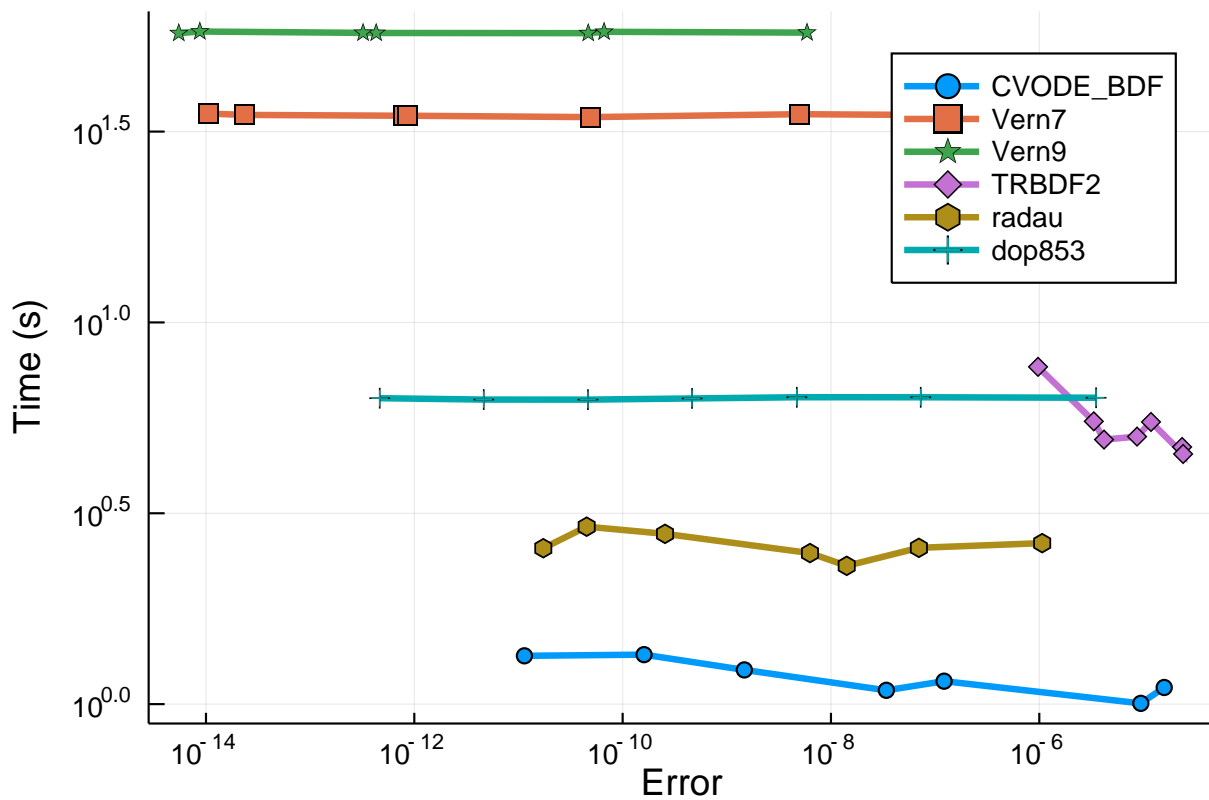
```

reltols=1 ./10 .^(6:12)
setup = [
    Dict(:alg => CVODE_BDF()),
    Dict(:alg => Vern7()),
    Dict(:alg => Vern9()),
    Dict(:alg => TRBDF2(autodiff=false)),
    Dict(:alg => radau()),
    Dict(:alg => dop853())
];

names = [
    "CVODE_BDF",
    "Vern7",
    "Vern9",
    "TRBDF2",
    "radau",
    "dop853"
];

wp = WorkPrecisionSet(prob, abstols, reltols, setup; names=names, appxsol=test_sol,
    maxiters=Int(1e6), verbose = false)
plot(wp)

```



```

abstols=1 ./10 .^(6:12)
reltols=1 ./10 .^(6:12)
setup = [
    Dict(:alg => CVODE_BDF()),
    Dict(:alg => radau()),
    Dict(:alg => TRBDF2(autodiff=false)),
    Dict(:alg => Kvaerno3(autodiff=false)),
    Dict(:alg => KenCarp3(autodiff=false)),
    Dict(:alg => Kvaerno4(autodiff=false)),
    Dict(:alg => KenCarp4(autodiff=false)),

```

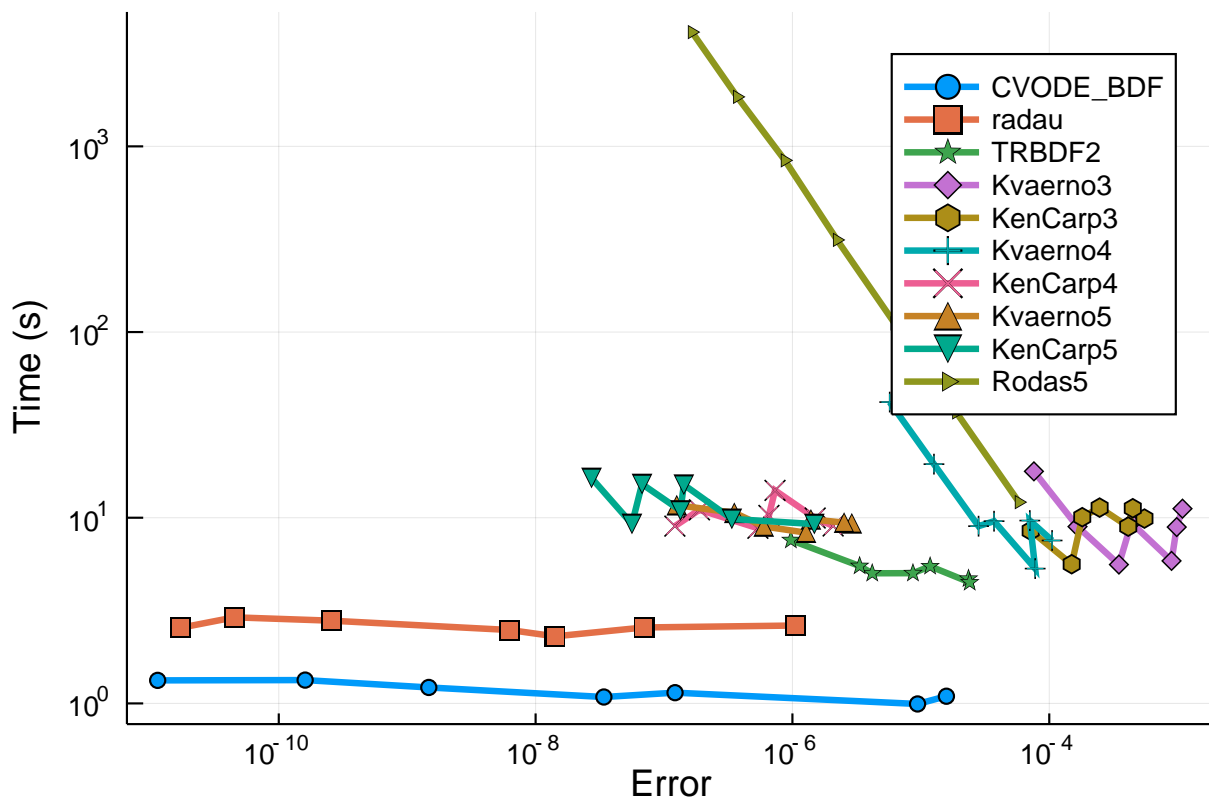
```

Dict(:alg => Kvaerno5(autodiff=false)),
Dict(:alg => KenCarp5(autodiff=false)),
Dict(:alg => Rodas5(autodiff=false)),
#Dict(:alg => lsoda())
];

names = [
  "CVODE_BDF",
  "radau",
  "TRBDF2",
  "Kvaerno3",
  "KenCarp3",
  "Kvaerno4",
  "KenCarp4",
  "Kvaerno5",
  "KenCarp5",
  "Rodas5",
  #"lsoda"
];

wp = WorkPrecisionSet(prob, abstols, reltols, setups; names=names, appxsol=test_sol,
  maxiters=Int(1e6), verbose = false)
plot(wp)

```



By looking at the previous plots, we can see that KenCarp3 is the quicker one and lsoda is the slower one (the colors are similar!)

3.2.1 Timeseries Error

```

abstols=1 ./10 .^(6:12)
reltols=1 ./10 .^(6:12)
setups = [

```



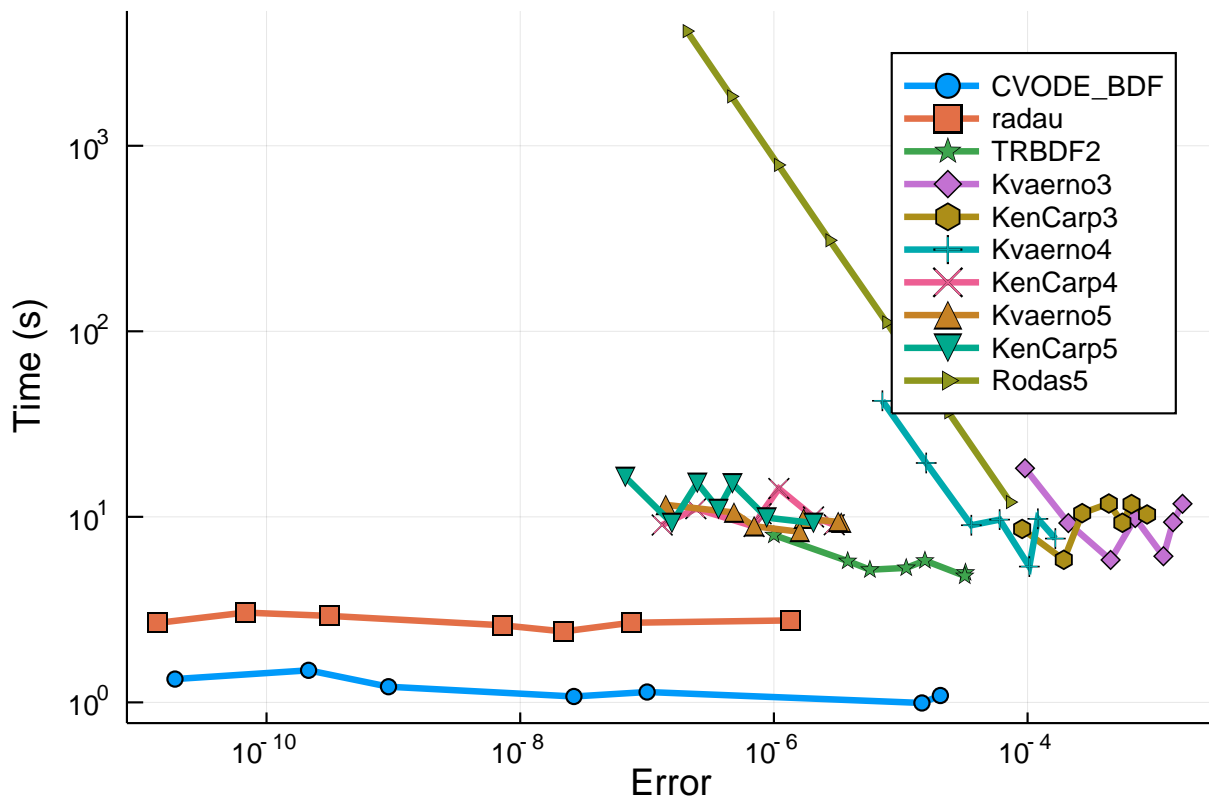
```

Dict(:alg => CVODE_BDF()),
Dict(:alg => radau()),
Dict(:alg => TRBDF2(autodiff=false)),
Dict(:alg => Kvaerno3(autodiff=false)),
Dict(:alg => KenCarp3(autodiff=false)),
Dict(:alg => Kvaerno4(autodiff=false)),
Dict(:alg => KenCarp4(autodiff=false)),
Dict(:alg => Kvaerno5(autodiff=false)),
Dict(:alg => KenCarp5(autodiff=false)),
Dict(:alg => Rodas5(autodiff=false)),
#Dict(:alg => lsoda())
];

names = [
  "CVODE_BDF",
  "radau",
  "TRBDF2",
  "Kvaerno3",
  "KenCarp3",
  "Kvaerno4",
  "KenCarp4",
  "Kvaerno5",
  "KenCarp5",
  "Rodas5",
  #"lsoda"
];

wp = WorkPrecisionSet(prob, abstols, reltols, setups; names=names, appxsol=test_sol,
  maxiters=Int(1e6), verbose = false, error_estimate = :l2)
plot(wp)

```



3.2.2 Dense Error

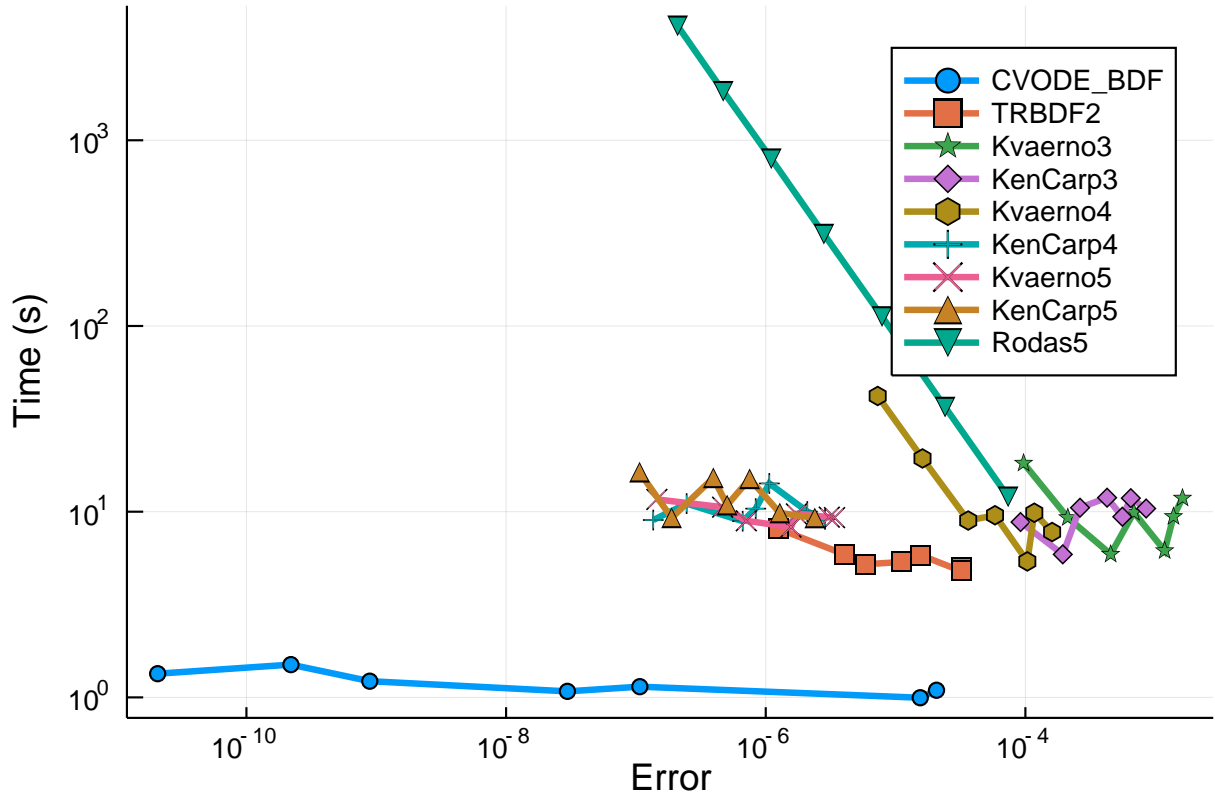
```

abstols=1 ./10 .^(6:12)
reltols=1 ./10 .^(6:12)
setups = [
    Dict(:alg => CVODE_BDF()),
    Dict(:alg => TRBDF2(autodiff=false)),
    Dict(:alg => Kvaerno3(autodiff=false)),
    Dict(:alg => KenCarp3(autodiff=false)),
    Dict(:alg => Kvaerno4(autodiff=false)),
    Dict(:alg => KenCarp4(autodiff=false)),
    Dict(:alg => Kvaerno5(autodiff=false)),
    Dict(:alg => KenCarp5(autodiff=false)),
    Dict(:alg => Rodas5(autodiff=false)),
];

names = [
    "CVODE_BDF",
    "TRBDF2",
    "Kvaerno3",
    "KenCarp3",
    "Kvaerno4",
    "KenCarp4",
    "Kvaerno5",
    "KenCarp5",
    "Rodas5"
];

wp = WorkPrecisionSet(prob, abstols, reltols, setups; names=names, appxsol=test_sol,
    maxiters=Int(1e6), verbose = false, dense_errors=true,
    error_estimate = :L2)
plot(wp)

```



4 No Jacobian Work-Precision Diagrams

In the previous cases the analytical Jacobian is given and is used by the solvers. Now we will solve the same problem without the analytical Jacobian.

Note that the pre-caching means that the model is not compatible with autodifferentiation by ForwardDiff. Thus all of the native Julia solvers are set to `autodiff=false` to use DiffEqDiffTools.jl's numerical differentiation backend. We'll only benchmark the methods that did well before.

```
N=20
f = FilamentCache(N, Solver=SolverDiffEq)
r0 = initialize!(StraightX, f)
stiffness_matrix!(f)
prob = ODEProblem(ODEFunction(f, jac=nothing), r0, (0., 0.01))

sol = solve(prob, Vern9(), reltol=1e-14, abstol=1e-14)
test_sol = TestSolution(sol.t, sol.u);
```

4.1 High Tolerance (Low Accuracy)

```
abstols=1 ./10 .^(3:8)
reltols=1 ./10 .^(3:8)
setups = [
    Dict(:alg => CVODE_BDF()),
    Dict(:alg => TRBDF2(autodiff=false)),
    Dict(:alg => rodas()),
    Dict(:alg => radau()),
    Dict(:alg => KenCarp3(autodiff=false)),
```

```

Dict(:alg => Kvaerno4(autodiff=false)),
Dict(:alg => ROCK2()),
Dict(:alg => ROCK4())
];

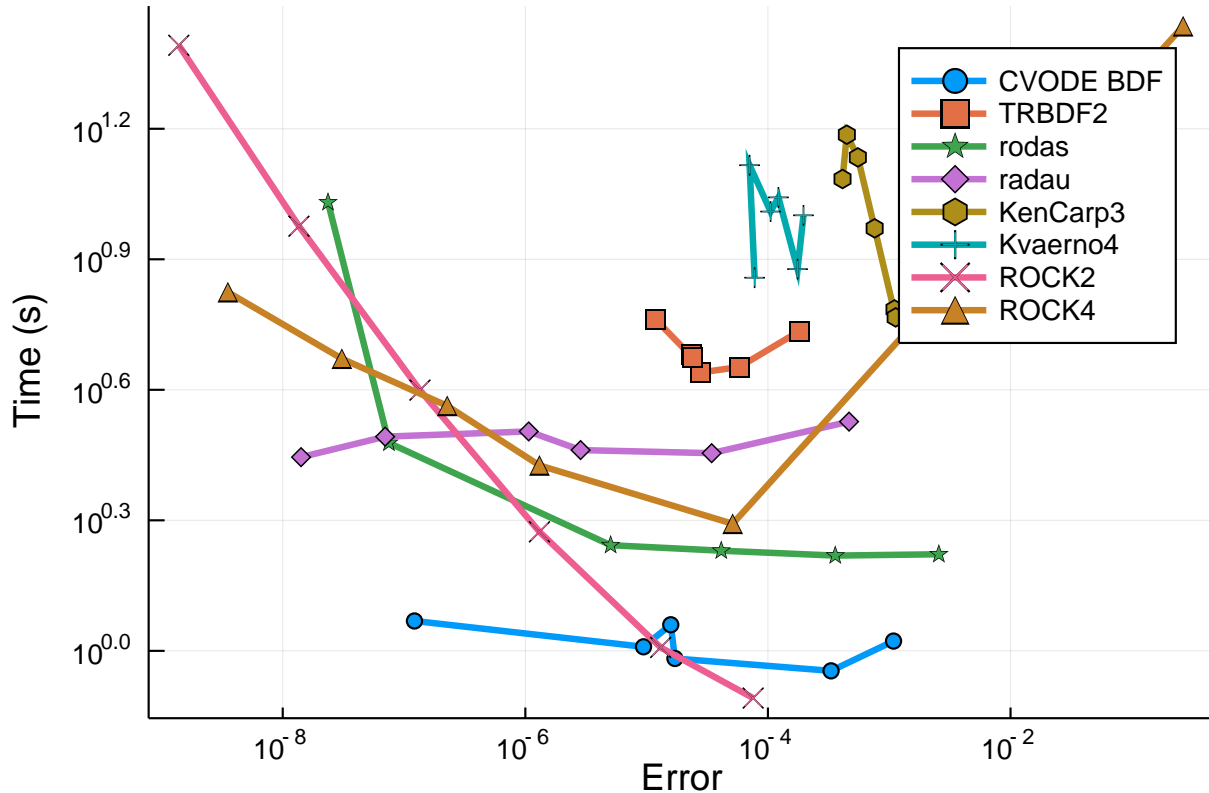
names = [
  "CVODE BDF",
  "TRBDF2",
  "rodas",
  "radau",
  "KenCarp3",
  "Kvaerno4",
  "ROCK2",
  "ROCK4"
];

wp = WorkPrecisionSet(prob, abstols, reltols, setups; names=names, appxsol=test_sol,
  maxiters=Int(1e6), verbose = true, numruns = 10)

EXIT OF RADAU AT X=      0.1000E-01
STEP SIZE TOO SMALL, H= 1.7347234759768071E-018
EXIT OF RADAU AT X=      0.1000E-01
STEP SIZE TOO SMALL, H= 1.7347234759768071E-018
EXIT OF RADAU AT X=      0.1000E-01
STEP SIZE TOO SMALL, H= 1.7347234759768071E-018

plot(wp)

```



It looks like `radau` fails on this problem with low accuracy if the Jacobian is not passed, so its values should be ignored since it exits early.

```
abstols=1 ./10 .^(3:8)
```

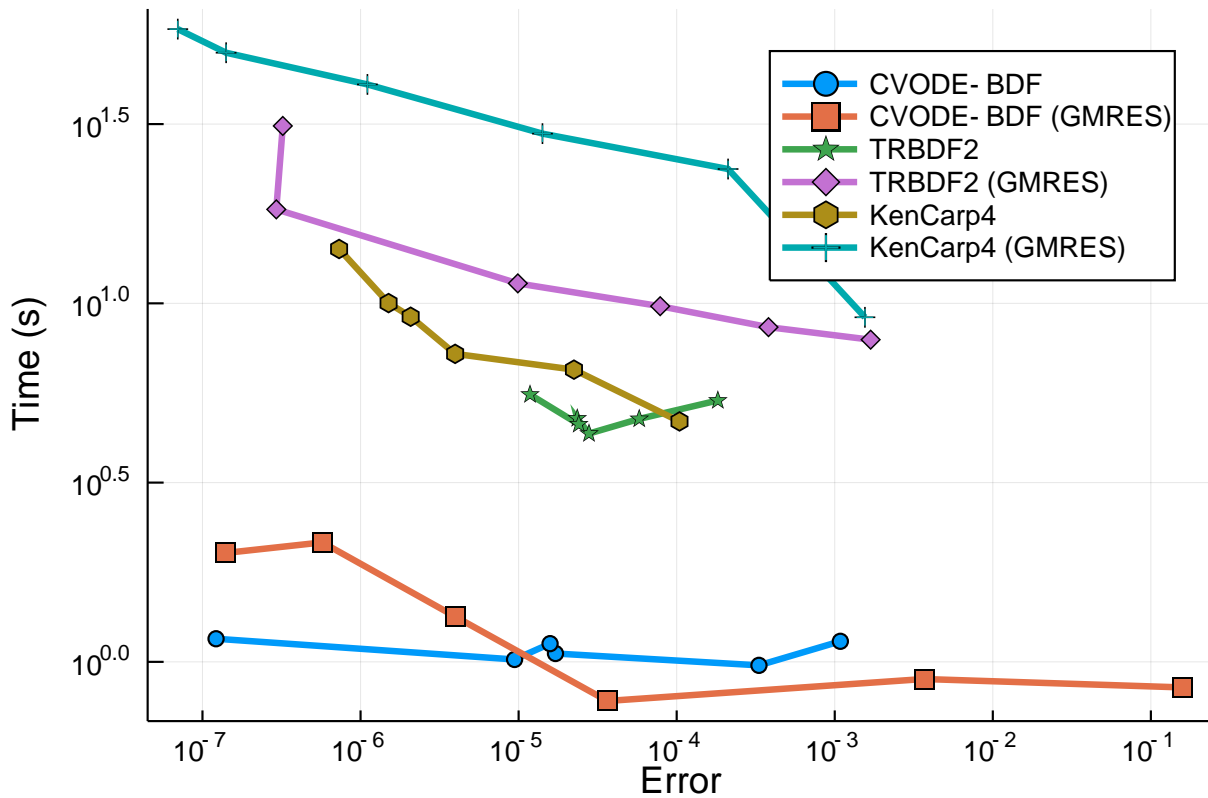
```

reltols=1 ./10 .^(3:8)
setups = [
    Dict(:alg => CVMODE_BDF()),
    Dict(:alg => CVMODE_BDF(linear_solver=:GMRES)),
    Dict(:alg => TRBDF2(autodiff=false)),
    Dict(:alg => TRBDF2(autodiff=false,linsolve=LinSolveGMRES())),
    Dict(:alg => KenCarp4(autodiff=false)),
    Dict(:alg => KenCarp4(autodiff=false,linsolve=LinSolveGMRES())),
];

names = [
    "CVMODE-BDF",
    "CVMODE-BDF (GMRES)",
    "TRBDF2",
    "TRBDF2 (GMRES)",
    "KenCarp4",
    "KenCarp4 (GMRES)",
];

wp = WorkPrecisionSet(prob, abstols, reltols, setups; names=names, appxsol=test_sol,
    maxiters=Int(1e6), verbose = false)
plot(wp)

```



4.2 Low Tolerance (High Accuracy)

```

abstols=1 ./ 10 .^(6:12)
reltols=1 ./ 10 .^(6:12)
setups = [
    Dict(:alg => CVMODE_BDF()),
    Dict(:alg => TRBDF2(autodiff=false)),
    Dict(:alg => rodas()),
];

```

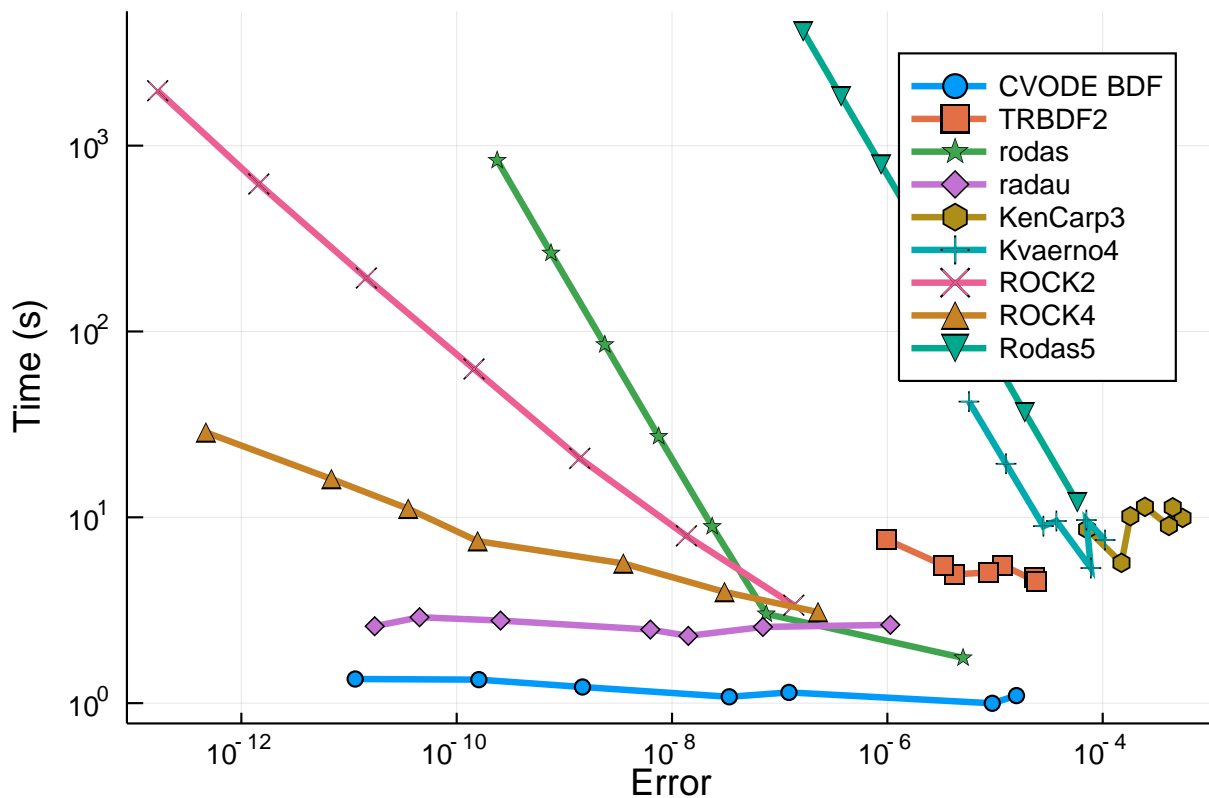
```

Dict(:alg => radau()),
Dict(:alg => KenCarp3(autodiff=false)),
Dict(:alg => Kvaerno4(autodiff=false)),
Dict(:alg => ROCK2()),
Dict(:alg => ROCK4()),
Dict(:alg => Rodas5(autodiff=false)),
];

names = [
  "CVODE BDF",
  "TRBDF2",
  "rodas",
  "radau",
  "KenCarp3",
  "Kvaerno4",
  "ROCK2",
  "ROCK4",
  "Rodas5"
];

wp = WorkPrecisionSet(prob, abstols, reltols, setups; names=names, appxsol=test_sol,
  maxiters=Int(1e6), verbose = true, numruns = 10)
plot(wp)

```



4.3 Conclusion

Sundials' CVODE_BDF does the best in this test. When the Jacobian is given, the ESDIRK methods TRBDF2 and KenCarp3 are able to do almost as well as it until $<1e-6$ error is needed. When Jacobians are not given, Sundials is the fastest without competition.

using DiffEqBenchmarks

```
DiffEqBenchmarks.bench_footer(WEAVE_ARGS[:folder],WEAVE_ARGS[:file])
```

4.4 Appendix

These benchmarks are a part of the DiffEqBenchmarks.jl repository, found at: <https://github.com/JuliaDiffEq/DiffEqBenchmarks.jl>

To locally run this tutorial, do the following commands:

```
using DiffEqBenchmarks
DiffEqBenchmarks.weave_file("MOLPDE","Filament.jmd")
```

Computer Information:

```
Julia Version 1.1.0
Commit 80516ca202 (2019-01-21 21:24 UTC)
Platform Info:
  OS: Linux (x86_64-pc-linux-gnu)
  CPU: Intel(R) Xeon(R) CPU E5-2680 v4 @ 2.40GHz
  WORD_SIZE: 64
  LIBM: libopenlibm
  LLVM: libLLVM-6.0.1 (ORCJIT, haswell)
```

Package Information:

```
Status: `~/home/crackauckas/.julia/environments/v1.1/Project.toml`
[c52e3926-4ff0-5f6e-af25-54175e0327b1] Atom 0.8.8
[bcd4f6db-9728-5f36-b5f7-82caef46ccdb] DelayDiffEq 5.9.1
[bb2cbb15-79fc-5d1e-9bf1-8ae49c7c1650] DiffEqBenchmarks 0.1.0
[459566f4-90b8-5000-8ac3-15dfb0a30def] DiffEqCallbacks 2.5.2
[f3b72e0c-5b89-59e1-b016-84e28bfd966d] DiffEqDevTools 2.13.0
[aae7a2af-3d4f-5e19-a356-7da93b79d9d0] DiffEqFlux 0.6.1
[78ddff82-25fc-5f2b-89aa-309469cbf16f] DiffEqMonteCarlo 0.15.1
[77a26b50-5914-5dd7-bc55-306e6241c503] DiffEqNoiseProcess 3.3.1
[9fdde737-9c7f-55bf-ade8-46b3f136cc48] DiffEqOperators 3.5.0
[055956cb-9e8b-5191-98cc-73ae4a59e68a] DiffEqPhysics 3.2.0
[a077e3f3-b75c-5d7f-a0c6-6bc4c8ec64a9] DiffEqProblemLibrary 4.5.0
[ef61062a-5684-51dc-bb67-a0fcdec5c97d] DiffEqUncertainty 1.1.0
[0c46a032-eb83-5123-abaf-570d42b7fbba] DifferentialEquations 6.6.0
[35a29f4d-8980-5a13-9543-d66fff28ecb8] DocumenterTools 0.1.1
[b305315f-e792-5b7a-8f41-49f472929428] Elliptic 0.5.0
[587475ba-b771-5e3f-ad9e-33799f191a9c] Flux 0.8.3
[e5e0dc1b-0480-54bc-9374-aad01c23163d] Juno 0.7.0
[7f56f5a3-f504-529b-bc02-0b1fe5e64312] LSODA 0.4.0
[c030b06c-0b6d-57c2-b091-7029874bd033] ODE 2.4.0
[54ca160b-1b9f-5127-a996-1867f4bc2a2c] ODEInterface 0.4.6
[09606e27-ecf5-54fc-bb29-004bd9f985bf] ODEInterfaceDiffEq 3.3.1
```

[1dea7af3-3e70-54e6-95c3-0bf5283fa5ed] OrdinaryDiffEq 5.12.0
[2dcacdae-9679-587a-88bb-8b444fb7085b] ParallelDataTransfer 0.5.0
[65888b18-ceab-5e60-b2b9-181511a3b968] ParameterizedFunctions 4.2.0
[91a5bcdd-55d7-5caf-9e0b-520d859cae80] Plots 0.26.0
[9cded84f-2146-5f9f-b71f-7cd68310d1ff] PumasDocs 0.0.0
[d330b81b-6aea-500a-939a-2ce795aea3ee] PyPlot 2.8.1
[731186ca-8d62-57ce-b412-fbd966d074cd] RecursiveArrayTools 0.20.0
[295af30f-e4ad-537b-8983-00126c2a3abe] Revise 2.1.6
[90137ffa-7385-5640-81b9-e52037218182] StaticArrays 0.11.0
[789caeaf-c7a9-5a7d-9973-96adeb23e2a0] StochasticDiffEq 6.6.0
[c3572dad-4567-51f8-b174-8c6c989267f4] Sundials 3.6.1
[92b13dbe-c966-51a2-8445-caca9f8a7d42] TaylorIntegration 0.5.0
[44d3d7a6-8a23-5bf8-98c5-b353f8df5ec9] Weave 0.9.1
[e88e6eb3-aa80-5325-afca-941959d7151f] Zygote 0.3.2