Allen-Cahn Pseudospectral Methods Work-Precision Diagrams

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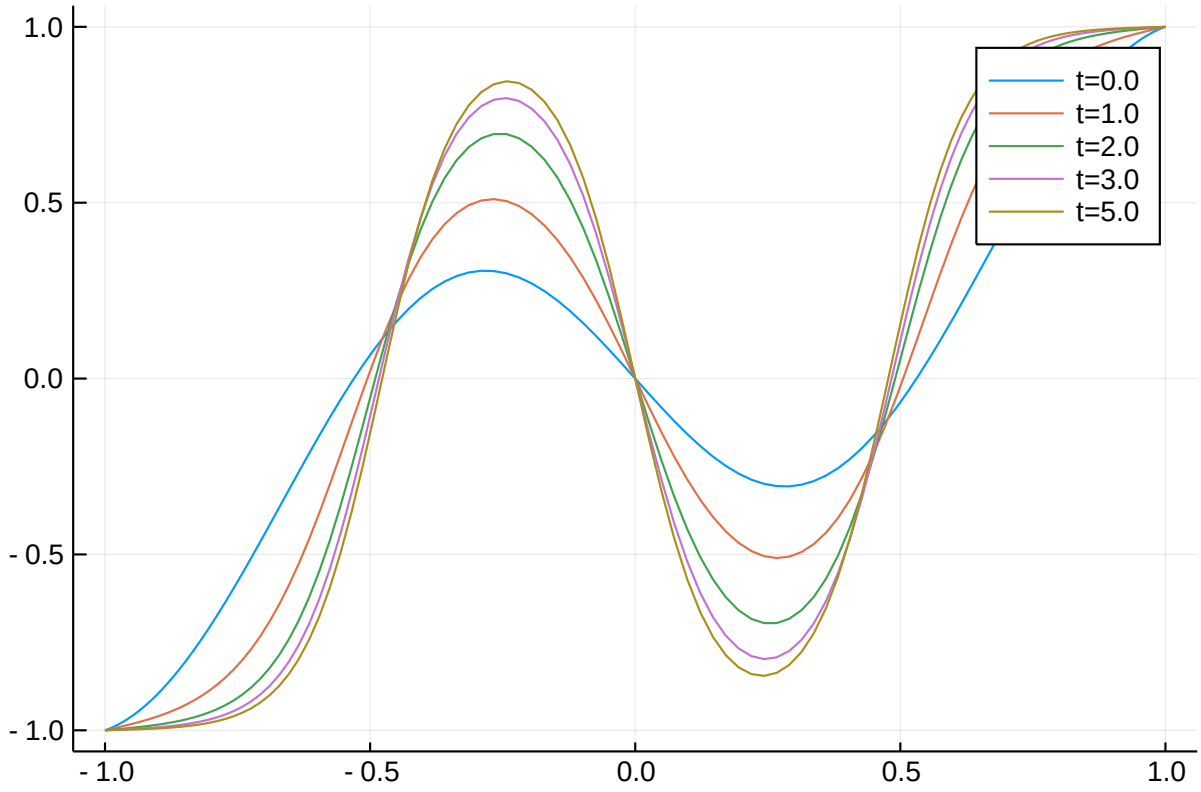
```
using ApproxFun, OrdinaryDiffEq, Sundials
using DiffEqDevTools
using LinearAlgebra
using Plots; gr()
```

Here is the Allen-Cahn equation using Chebyshev spectral methods.

```
function cheb(N)
    N==0 && return (0,1)
    x = cos.(pi*(0:N)/N)
    c = [2; ones(N-1,1); 2].*(-1).^(0:N)
    X = hcat([x for i in 1:N+1]...)
    dX = X-X'
    D  = (c*(1 ./c)')./(dX+I)      # off-diagonal entries
    D  = D .- Diagonal(vec(sum(D,dims=2)))                # diagonal entries
    D,x
end
N = 128
ChebD2,x = cheb(N)
xx = x
x = x[2:N]
w = .53*x + .47*sin.(-1.5*pi*x) - x # use w = u-x to make BCs homogeneous
u = [1;w+x;-1]

ϵ=0.01
D2=ϵ*(ChebD2^2)[2:N, 2:N]
function allen_cahn(du,u,x,t)
    @. du = (u + x) - (u + x)^3
end

allen_cahn (generic function with 1 method)
```

Reference solution using RadauIIA5 is below:

```
prob = SplitODEProblem(DiffEqArrayOperator(D2), allen_cahn, w, (0.0,5.0), x)
sol  = solve(prob, RadauIIA5(autodiff=false); reltol=1e-14,abstol=1e-14)
test_sol = TestSolution(sol)

tslices=[0.0 1.0 2.0 3.0 5.0]
ys=hcat(([1;x.+sol(t);-1] for t in tslices)...)
labels=["t=$t" for t in tslices]
plot(xx,ys,label=labels)
```



0.1 High tolerances

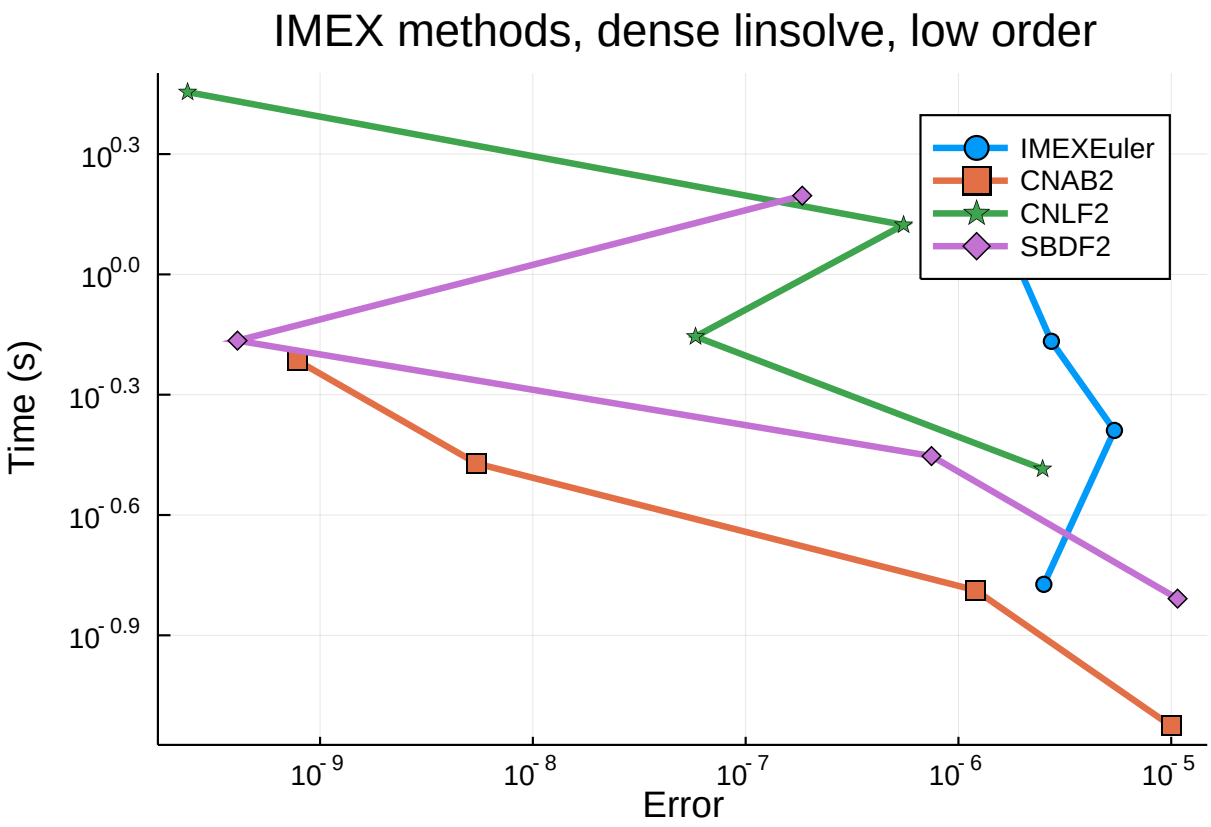
0.2 In-family comparisons

1.IMEX methods (dense linear solver)

```
abstols = 0.1 .^ (5:8)
reltols = 0.1 .^ (1:4)
multipliers =  0.5 .^ (0:3)
setups = [Dict(:alg => IMEXEuler(), :dts => 1e-3 * multipliers),
          Dict(:alg => CNAB2(), :dts => 5e-3 * multipliers),
          Dict(:alg => CNLF2(), :dts => 5e-4 * multipliers),
          Dict(:alg => SBDF2(), :dts => 1e-3 * multipliers)]
labels = ["IMEXEuler" "CNAB2" "CNLF2" "SBDF2"]
@time wp1 = WorkPrecisionSet(prob,abstols,reltols,setups;
                             print_names=true,names=labels,
                             numruns=5,seconds=5,
                             save_everystop=false,appxsol=test_sol,maxiters=Int(1e5));
```

```
IMEXEuler
CNAB2
CNLF2
SBDF2
 93.774204 seconds (190.72 M allocations: 10.710 GiB, 2.18% gc time)
```

```
plot(wp1,label=labels,markershape=:auto,title="IMEX methods, dense linsolve, low order")
```

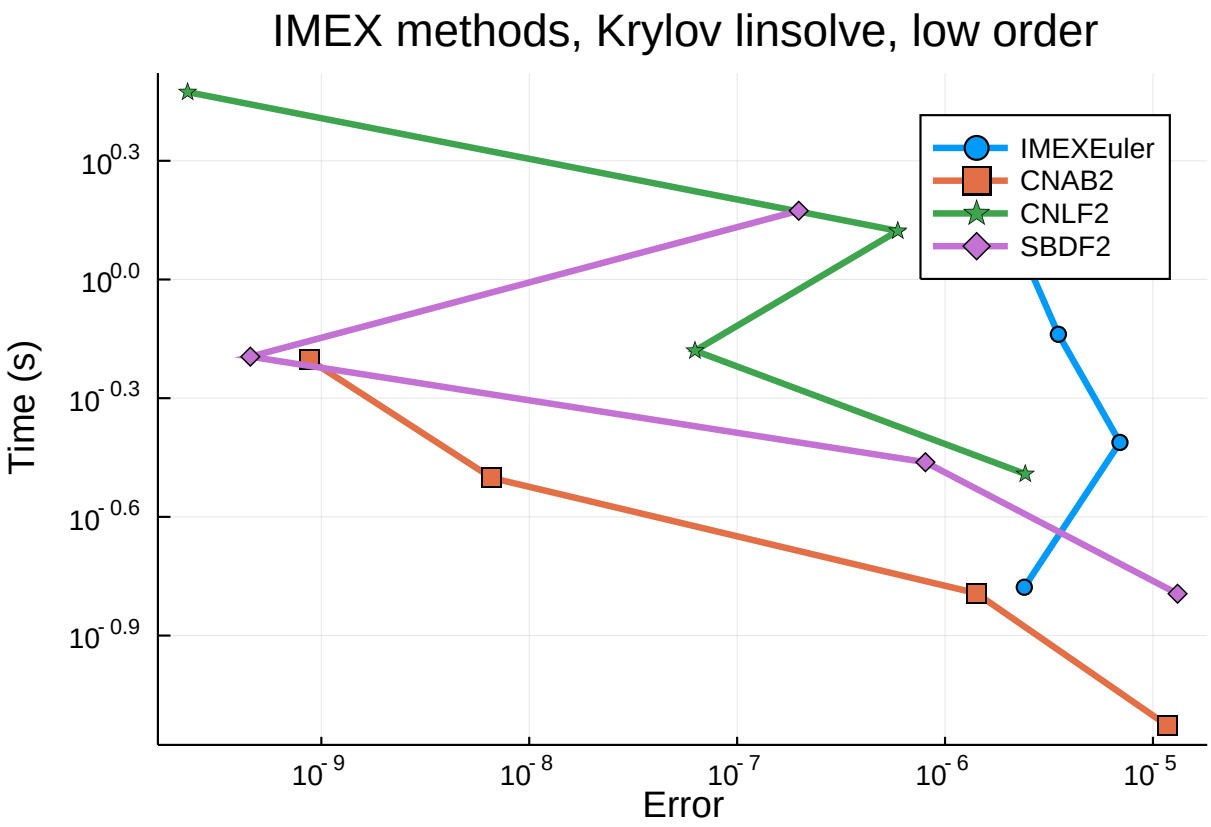


1.IMEX methods (Krylov linear solver)

```
abstols = 0.1 .^ (5:8) # all fixed dt methods so these don't matter much
reltols = 0.1 .^ (1:4)
multipliers = 0.5 .^ (0:3)
setups = [Dict(:alg => IMEXEuler(linsolve=LinSolveGMRES()), :dts => 1e-3 * multipliers),
          Dict(:alg => CNAB2(linsolve=LinSolveGMRES()), :dts => 5e-3 * multipliers),
          Dict(:alg => CNLF2(linsolve=LinSolveGMRES()), :dts => 5e-4 * multipliers),
          Dict(:alg => SBDF2(linsolve=LinSolveGMRES()), :dts => 1e-3 * multipliers)]
labels = ["IMEXEuler" "CNAB2" "CNLF2" "SBDF2"]
@time wp1 = WorkPrecisionSet(prob,abstols,reltols,setups;
                             print_names=true, names=labels,
                             numruns=5, error_estimate=:l2,
                             save_everystep=false, appxsol=test_sol, maxiters=Int(1e5));
```

```
IMEXEuler
CNAB2
CNLF2
SBDF2
 77.810757 seconds (142.92 M allocations: 6.127 GiB, 1.02% gc time)
```

```
plot(wp1, label=labels, markershape=:auto, title="IMEX methods, Krylov linsolve, low
order")
```

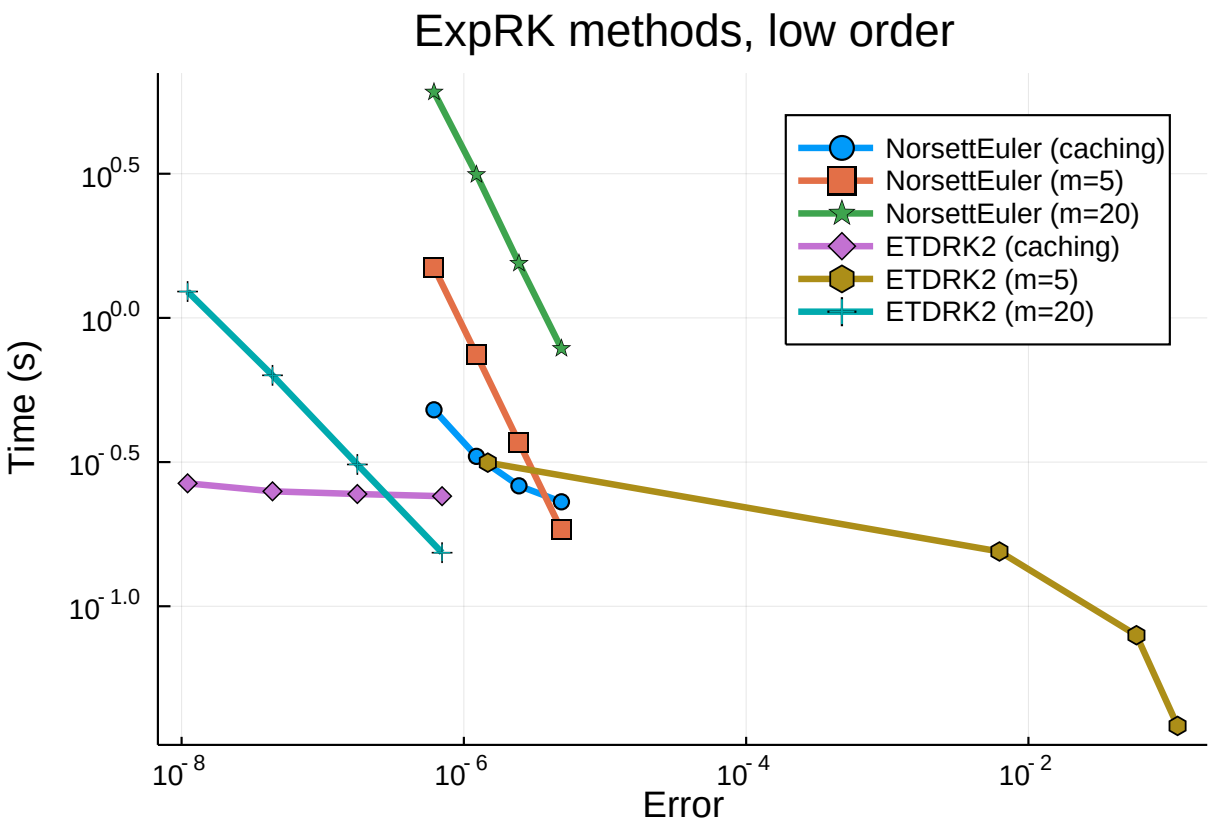


2. ExpRK methods

```
abstols = 0.1 .^ (5:8) # all fixed dt methods so these don't matter much
reltols = 0.1 .^ (1:4)
multipliers = 0.5 .^ (0:3)
setups = [Dict(:alg => NorsettEuler(), :dts => 1e-3 * multipliers),
          Dict(:alg => NorsettEuler(krylov=true, m=5), :dts => 1e-3 * multipliers),
          Dict(:alg => NorsettEuler(krylov=true, m=20), :dts => 1e-3 * multipliers),
          Dict(:alg => ETDRK2(), :dts => 1e-2 * multipliers),
          Dict(:alg => ETDRK2(krylov=true, m=5), :dts => 1e-2 * multipliers),
          Dict(:alg => ETDRK2(krylov=true, m=20), :dts => 1e-2 * multipliers)]
labels = hcat("NorsettEuler (caching)", "NorsettEuler (m=5)", "NorsettEuler (m=20)",
                            "ETDRK2 (caching)", "ETDRK2 (m=5)", "ETDRK2 (m=20)")
@time wp2 = WorkPrecisionSet(prob,abstols,reltols,setups;
                            print_names=true, names=labels,
                            numruns=5,
                            save_everystep=false, appxsol=test_sol, maxiters=Int(1e5));
```

```
NorsettEuler (caching)
NorsettEuler (m=5)
NorsettEuler (m=20)
ETDRK2 (caching)
ETDRK2 (m=5)
ETDRK2 (m=20)
105.768192 seconds (250.77 M allocations: 31.564 GiB, 2.34% gc time)
```

```
plot(wp2, label=labels, markershape=:auto, title="ExpRK methods, low order")
```

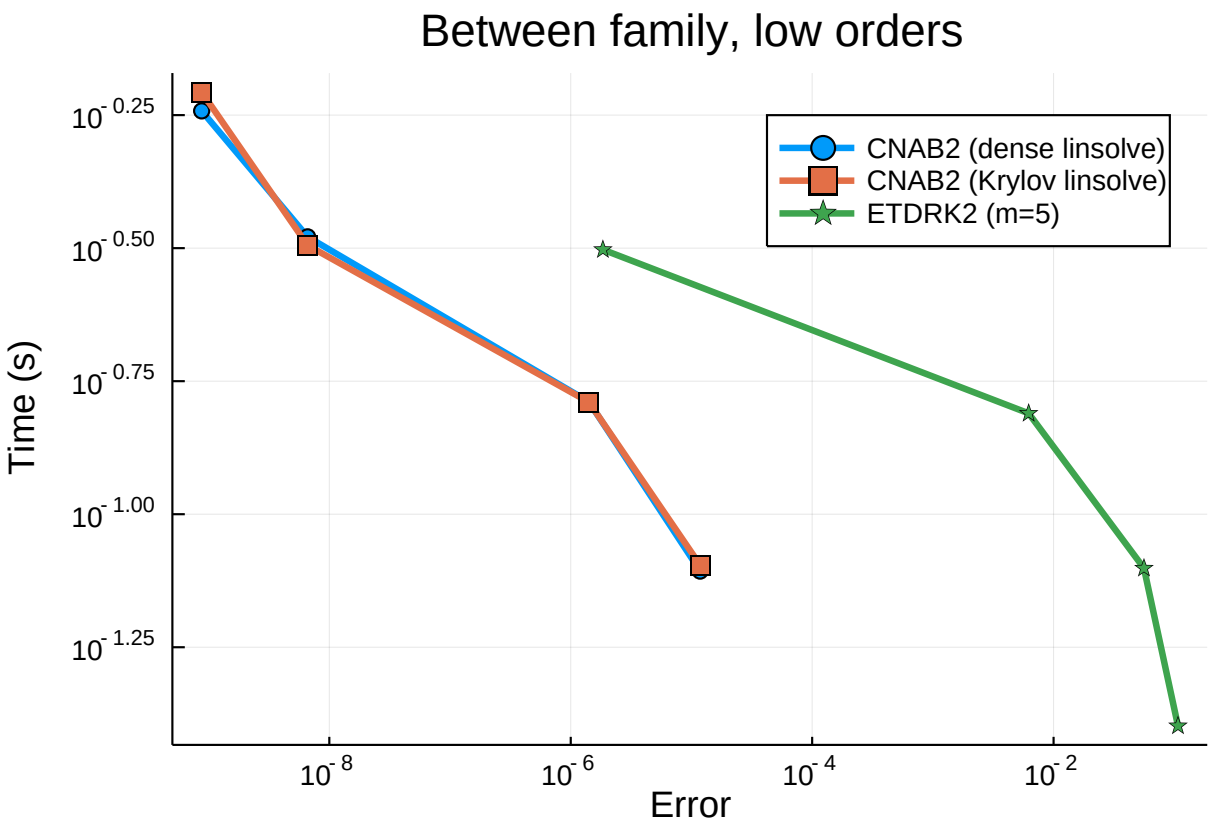


0.3 Between family comparisons

```
abstols = 0.1 .^ (5:8) # all fixed dt methods so these don't matter much
reltols = 0.1 .^ (1:4)
multipliers = 0.5 .^ (0:3)
setups = [Dict(:alg => CNAB2(), :dts => 5e-3 * multipliers),
          Dict(:alg => CNAB2(linsolve=LinSolveGMRES()), :dts => 5e-3 * multipliers),
          Dict(:alg => ETDRK2(krylov=true, m=5), :dts => 1e-2 * multipliers)]
labels = ["CNAB2 (dense linsolve)" "CNAB2 (Krylov linsolve)" "ETDRK2 (m=5)"]
@time wp3 = WorkPrecisionSet(prob,abstols,reltols,setups;
                             print_names=true, names=labels,
                             numruns=5, error_estimate=:l2,
                             save_everystep=false, appxsol=test_sol, maxiters=Int(1e5));
```

```
CNAB2 (dense linsolve)
CNAB2 (Krylov linsolve)
ETDRK2 (m=5)
 21.789528 seconds (42.01 M allocations: 2.240 GiB, 1.40% gc time)
```

```
plot(wp3, label=labels, markershape=:auto, title="Between family, low orders")
```



0.4 Low tolerances

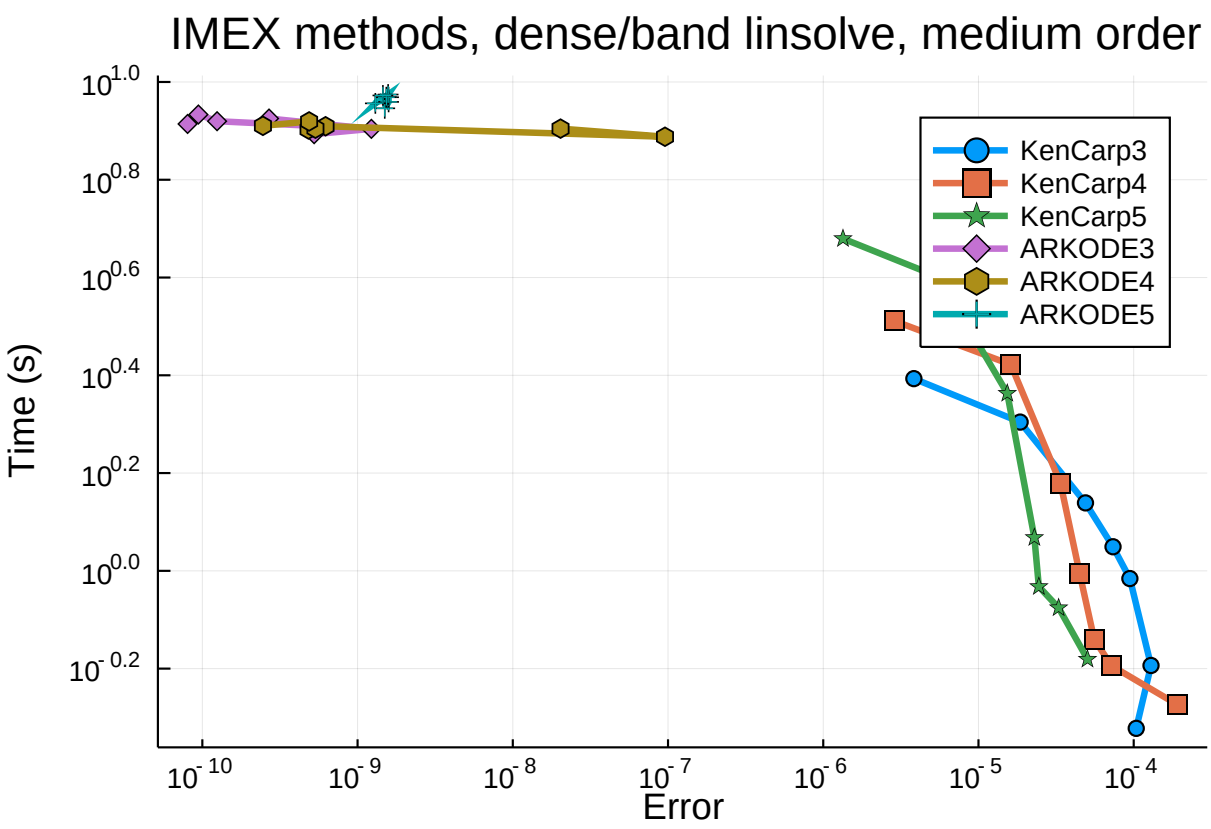
0.5 In-family comparisons

1.IMEX methods (dense/band linear solver)

```
abstols = 0.1 .^ (7:13)
reltols = 0.1 .^ (4:10)
setups = [Dict(:alg => KenCarp3()),
          Dict(:alg => KenCarp4()),
          Dict(:alg => KenCarp5()),
          Dict(:alg => ARKODE(Sundials.Implicit(), order=3, linear_solver=:Band,
jac_upper=1, jac_lower=1)),
          Dict(:alg => ARKODE(Sundials.Implicit(), order=4, linear_solver=:Band,
jac_upper=1, jac_lower=1)),
          Dict(:alg => ARKODE(Sundials.Implicit(), order=5, linear_solver=:Band,
jac_upper=1, jac_lower=1))]
labels = hcat("KenCarp3", "KenCarp4", "KenCarp5",
              "ARKODE3", "ARKODE4", "ARKODE5")
@time wp4 = WorkPrecisionSet(prob,abstols,reltols,setups;
                             print_names=true, names=labels,
                             numruns=5, error_estimate=:l2,
                             save_everystep=false, appxsol=test_sol, maxiters=Int(1e5));
```

```
KenCarp3
KenCarp4
KenCarp5
ARKODE3
ARKODE4
ARKODE5
700.221393 seconds (869.61 M allocations: 50.635 GiB, 1.12% gc time)
```

```
plot(wp4, label=labels, markershape=:auto, title="IMEX methods, dense/band linsolve,
medium order")
```

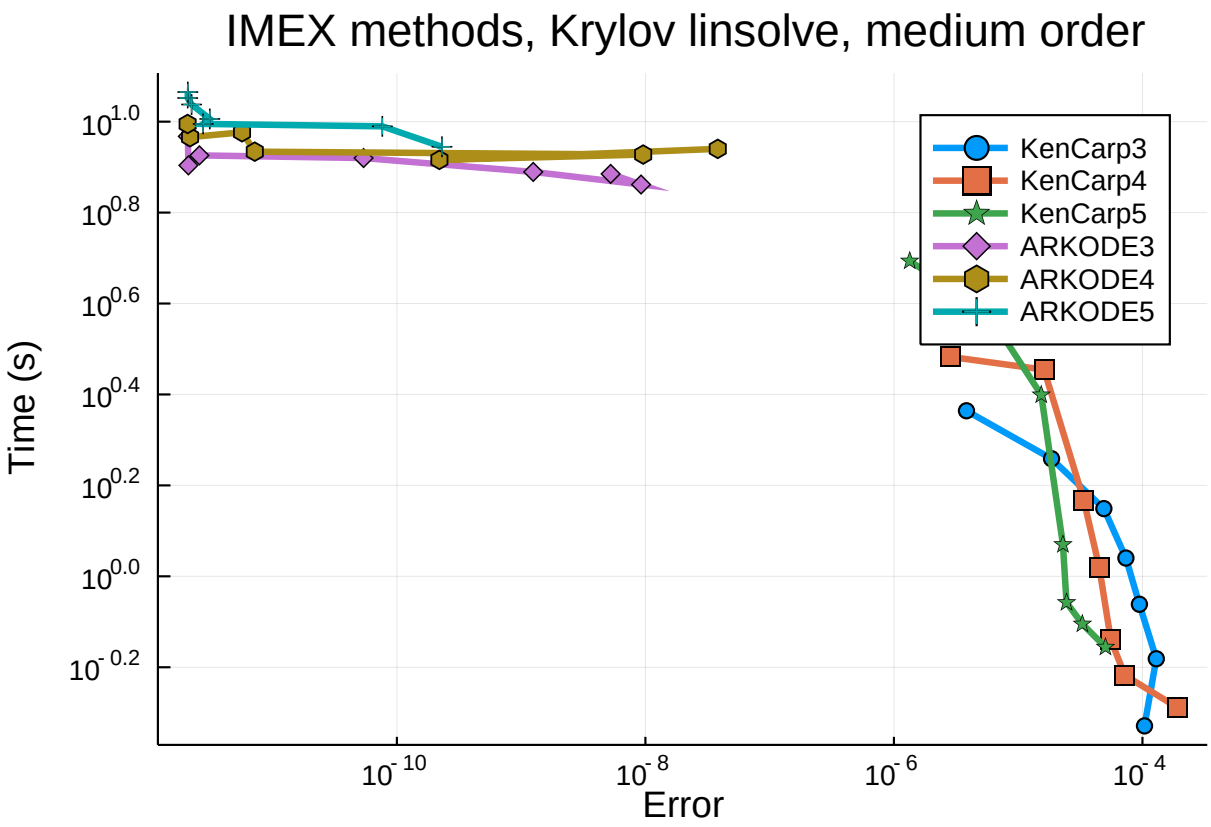


1.IMEX methods (krylov linear solver)

```
abstols = 0.1 .^ (7:13)
reltols = 0.1 .^ (4:10)
setups = [Dict(:alg => KenCarp3(linsolve=LinSolveGMRES())),
          Dict(:alg => KenCarp4(linsolve=LinSolveGMRES())),
          Dict(:alg => KenCarp5(linsolve=LinSolveGMRES())),
          Dict(:alg => ARKODE(Sundials.Implicit(), order=3, linear_solver=:GMRES)),
          Dict(:alg => ARKODE(Sundials.Implicit(), order=4, linear_solver=:GMRES)),
          Dict(:alg => ARKODE(Sundials.Implicit(), order=5, linear_solver=:GMRES))]
labels = ["KenCarp3" "KenCarp4" "KenCarp5" "ARKODE3" "ARKODE4" "ARKODE5"]
@time wp4 = WorkPrecisionSet(prob,abstols,reltols,setups;
                             print_names=true, names=labels,
                             numruns=5, error_estimate=:l2,
                             save_everystep=false, appxsol=test_sol, maxiters=Int(1e5));
```

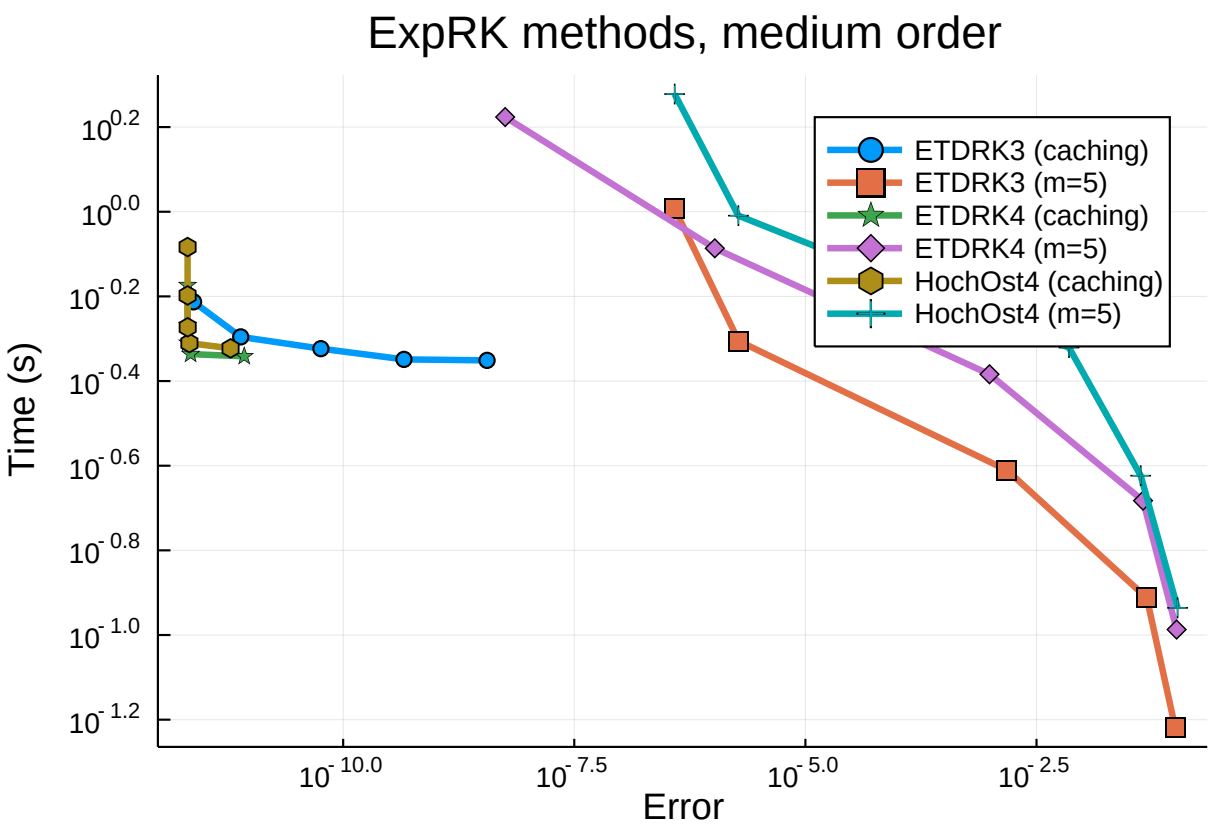
```
KenCarp3
KenCarp4
KenCarp5
ARKODE3
ARKODE4
ARKODE5
748.438970 seconds (1.09 G allocations: 66.982 GiB, 1.41% gc time)
```

```
plot(wp4, label=labels, markershape=:auto, title="IMEX methods, Krylov linsolve, medium
order")
```



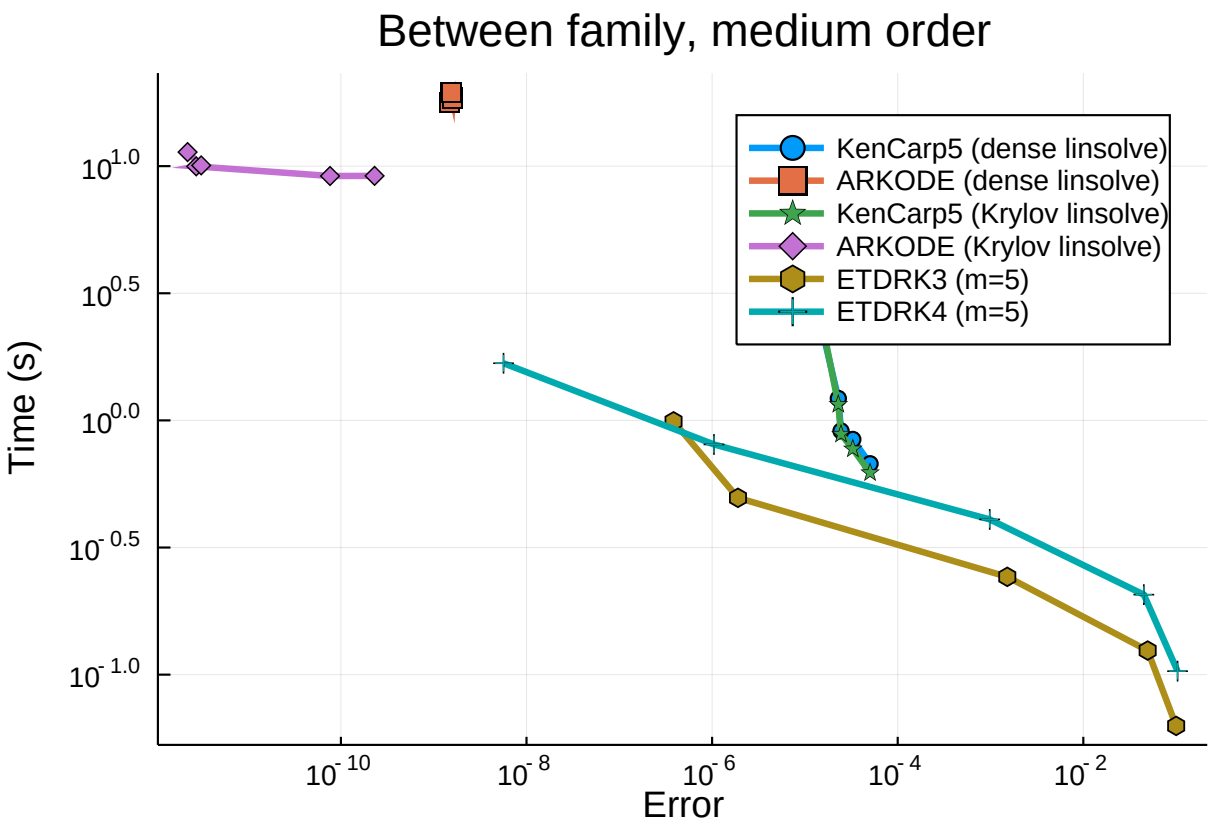
2.ExpRK methods

```
abstols = 0.1 .^ (7:11) # all fixed dt methods so these don't matter much
reltols = 0.1 .^ (4:8)
multipliers = 0.5 .^ (0:4)
setups = [Dict(:alg => ETDRK3(), :dts => 1e-2 * multipliers),
          Dict(:alg => ETDRK3(krylov=true, m=5), :dts => 1e-2 * multipliers),
          Dict(:alg => ETDRK4(), :dts => 1e-2 * multipliers),
          Dict(:alg => ETDRK4(krylov=true, m=5), :dts => 1e-2 * multipliers),
          Dict(:alg => HochOst4(), :dts => 1e-2 * multipliers),
          Dict(:alg => HochOst4(krylov=true, m=5), :dts => 1e-2 * multipliers)]
labels = hcat("ETDRK3 (caching)", "ETDRK3 (m=5)", "ETDRK4 (caching)",
              "ETDRK4 (m=5)", "HochOst4 (caching)", "HochOst4 (m=5)")
@time wp5 = WorkPrecisionSet(prob,abstols,reltols,setups;
                             print_names=true, names=labels,
                             numruns=5, error_estimate=:l2,
                             save_everystep=false, appxsol=test_sol, maxiters=Int(1e5));

ETDRK3 (caching)
ETDRK3 (m=5)
ETDRK4 (caching)
ETDRK4 (m=5)
HochOst4 (caching)
HochOst4 (m=5)
128.205894 seconds (163.55 M allocations: 34.587 GiB, 2.45% gc time)

plot(wp5, label=labels, markershape=:auto, title="ExpRK methods, medium order")
```



0.6 Between family comparisons

```
abstols = 0.1 .^ (7:11)
reltols = 0.1 .^ (4:8)
multipliers = 0.5 .^ (0:4)
setups = [Dict(:alg => KenCarp5()),
          Dict(:alg => ARKODE(Sundials.Implicit(), order=5, linear_solver=:Dense)),
          Dict(:alg => KenCarp5(linsolve=LinSolveGMRES())),
          Dict(:alg => ARKODE(Sundials.Implicit(), order=5, linear_solver=:GMRES)),
          Dict(:alg => ETDRK3(krylov=true, m=5), :dts => 1e-2 * multipliers),
          Dict(:alg => ETDRK4(krylov=true, m=5), :dts => 1e-2 * multipliers)]
labels = hcat("KenCarp5 (dense linsolve)", "ARKODE (dense linsolve)", "KenCarp5 (Krylov
linsolve)",
              "ARKODE (Krylov linsolve)", "ETDRK3 (m=5)", "ETDRK4 (m=5)")
@time wp6 = WorkPrecisionSet(prob,abstols,reltols,setups;
                             print_names=true, names=labels,
                             numruns=5, error_estimate=:l2,
                             save_everystep=false, appxsol=test_sol, maxiters=Int(1e5));

KenCarp5 (dense linsolve)
ARKODE (dense linsolve)
KenCarp5 (Krylov linsolve)
ARKODE (Krylov linsolve)
ETDRK3 (m=5)
ETDRK4 (m=5)
538.382017 seconds (537.45 M allocations: 37.447 GiB, 1.08% gc time)

plot(wp6, label=labels, markershape=:auto, title="Between family, medium order")
```




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

0.7 Appendix

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

To locally run this tutorial, do the following commands:

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

Computer Information:

```
Julia Version 1.3.0
Commit 46ce4d7933 (2019-11-26 06:09 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-6.0.1 (ORCJIT, skylake)
Environment:
  JULIA_NUM_THREADS = 8
```

Package Information:

```
Status: `/home/chrisrackauckas/.julia/dev/DiffEqBenchmarks/Project.toml`
```