Allen-Cahn Pseudospectral Methods Work-Precision Diagrams

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```
using ApproxFun, OrdinaryDiffEq, Sundials, BenchmarkTools, DiffEqOperators
```

```
Error: ArgumentError: Package DiffEqOperators not found in current path:
- Run `import Pkg; Pkg.add("DiffEqOperators")` to install the DiffEqOperato
rs package.
```

```
using DiffEqDevTools
using LinearAlgebra
using Plots; gr()
```

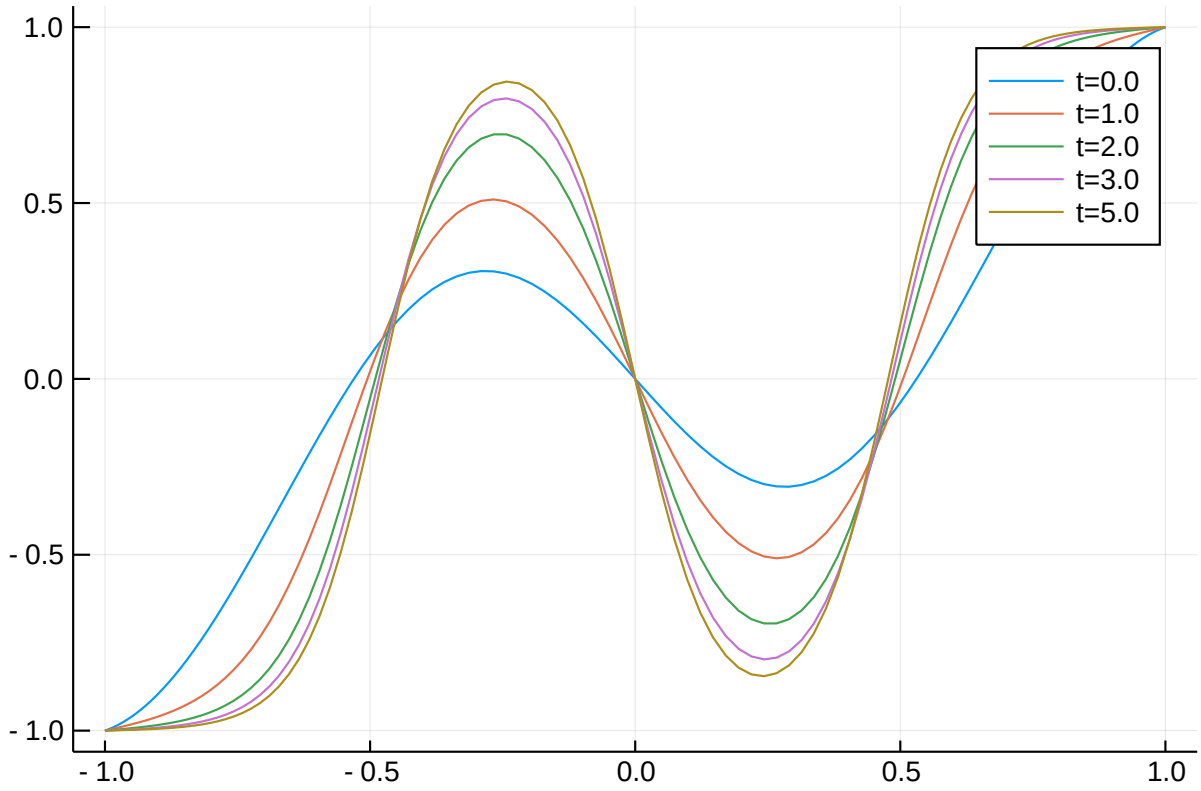
Here is the Allen-Cahn equation using Chebyshev spectral methods.

```
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

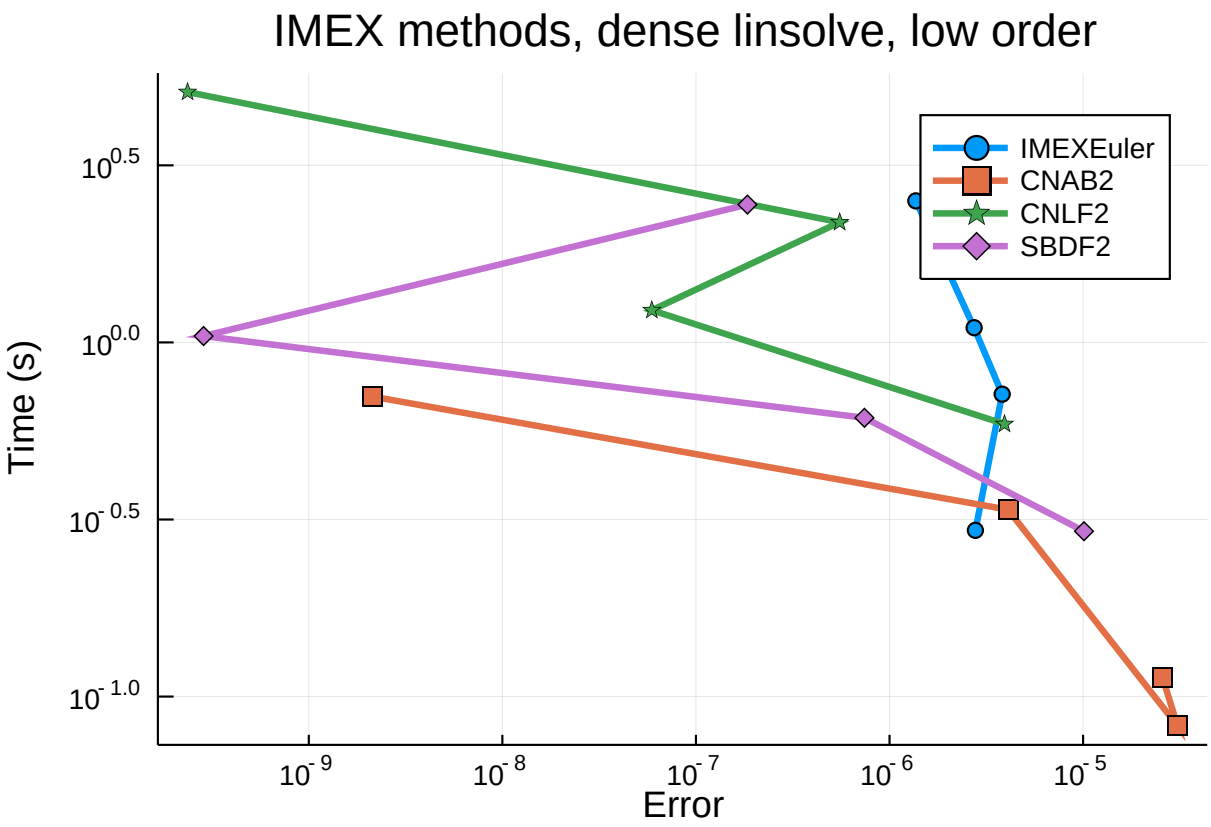
0.2 In-family comparisons

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
144.923779 seconds (153.09 M allocations: 9.145 GiB, 11.54% gc time)
```

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

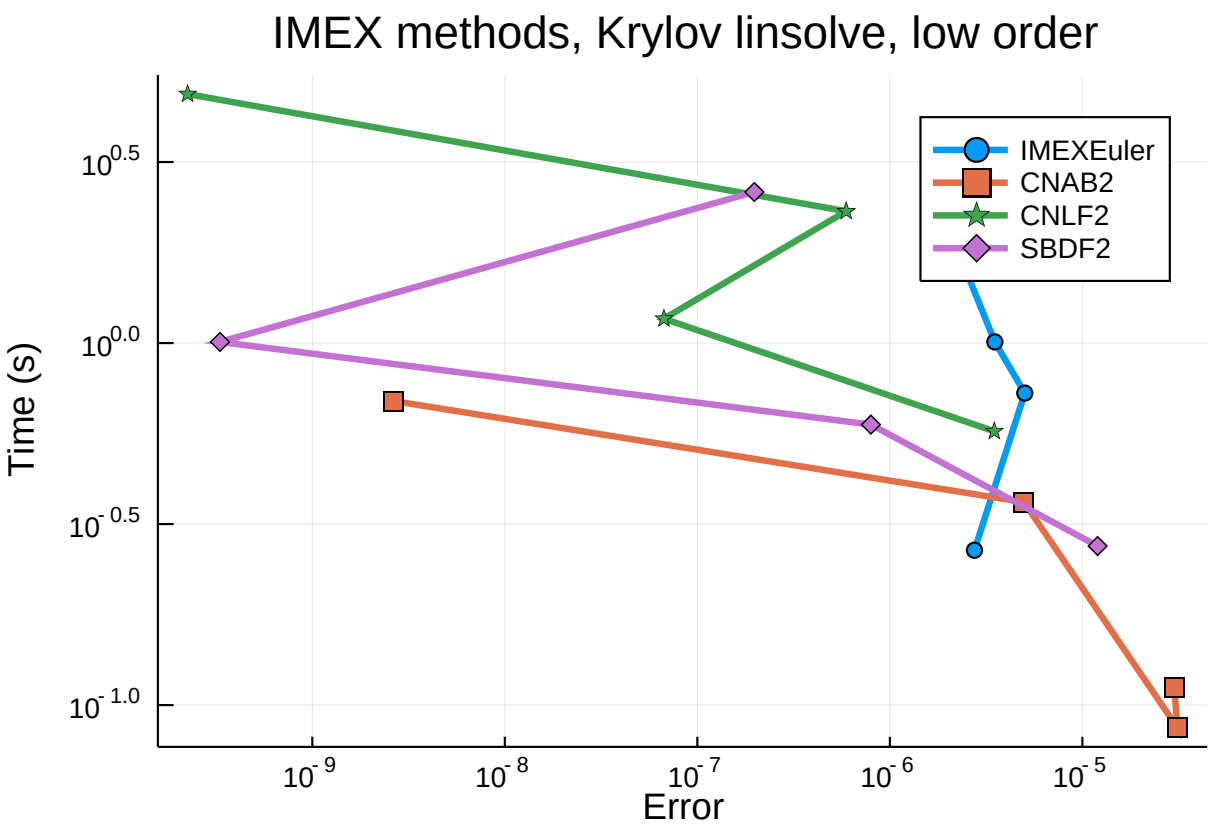


1.IMEX methods (Krylov linear solver)

```
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));
```

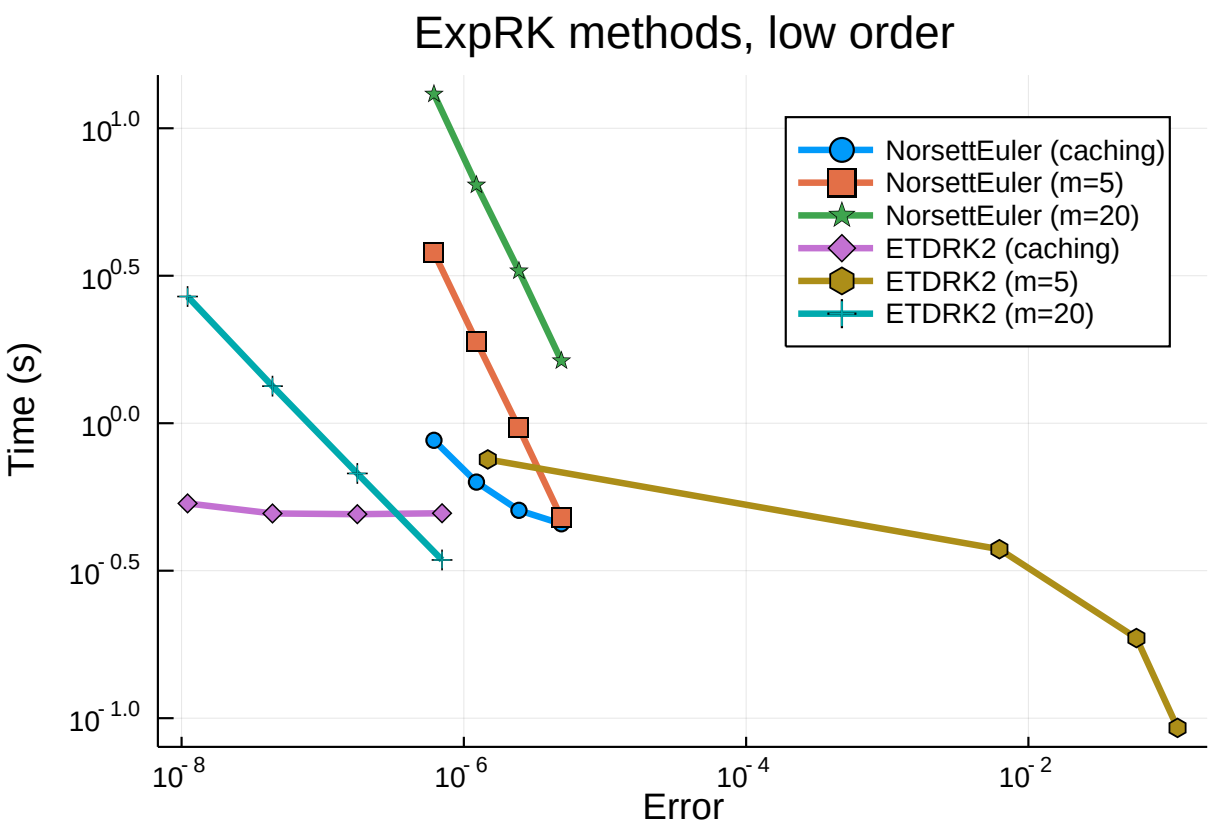
```
IMEXEuler
CNAB2
CNLF2
SBDF2
 95.017480 seconds (97.16 M allocations: 4.193 GiB, 4.55% gc time)
```

```
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)
192.875756 seconds (205.17 M allocations: 26.448 GiB, 7.86% gc time)

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

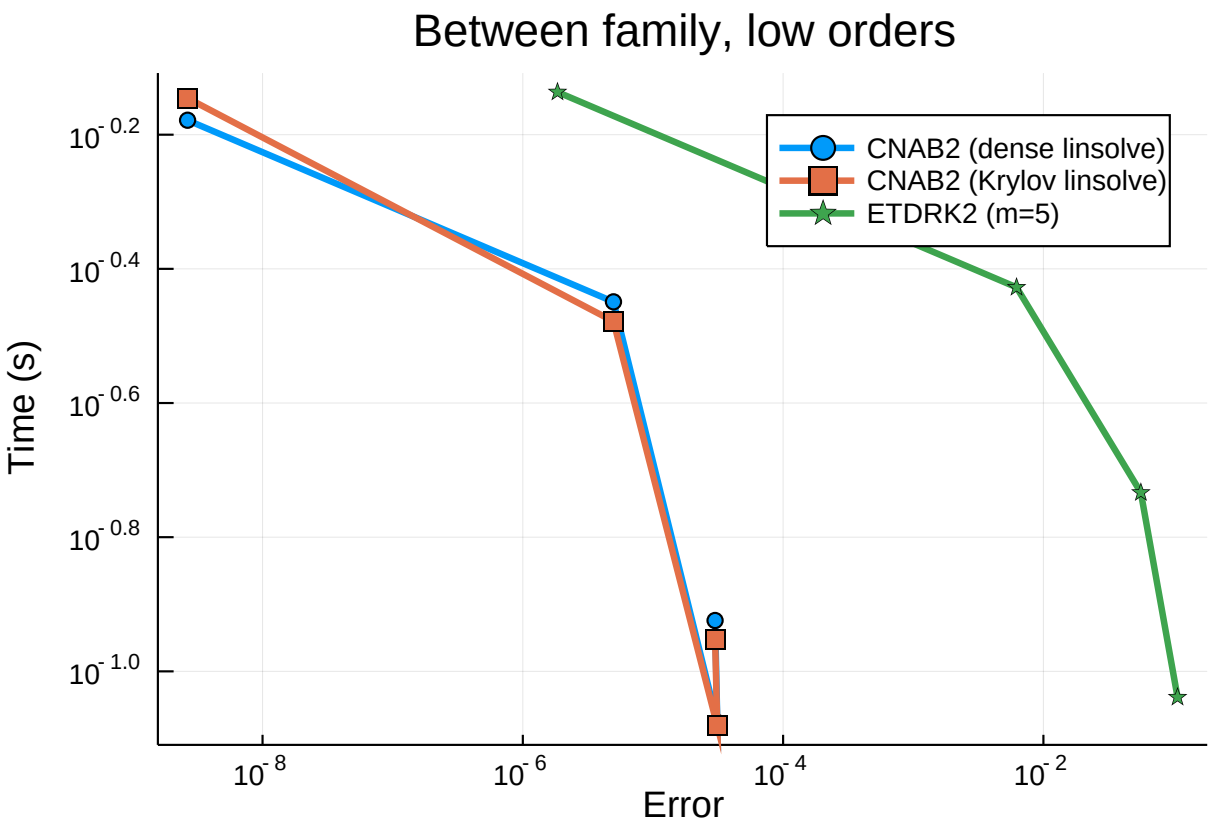


0.3 Between family comparisons

```
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)
 28.778954 seconds (26.27 M allocations: 1.576 GiB, 3.31% gc time)
```

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



0.4 Low tolerances

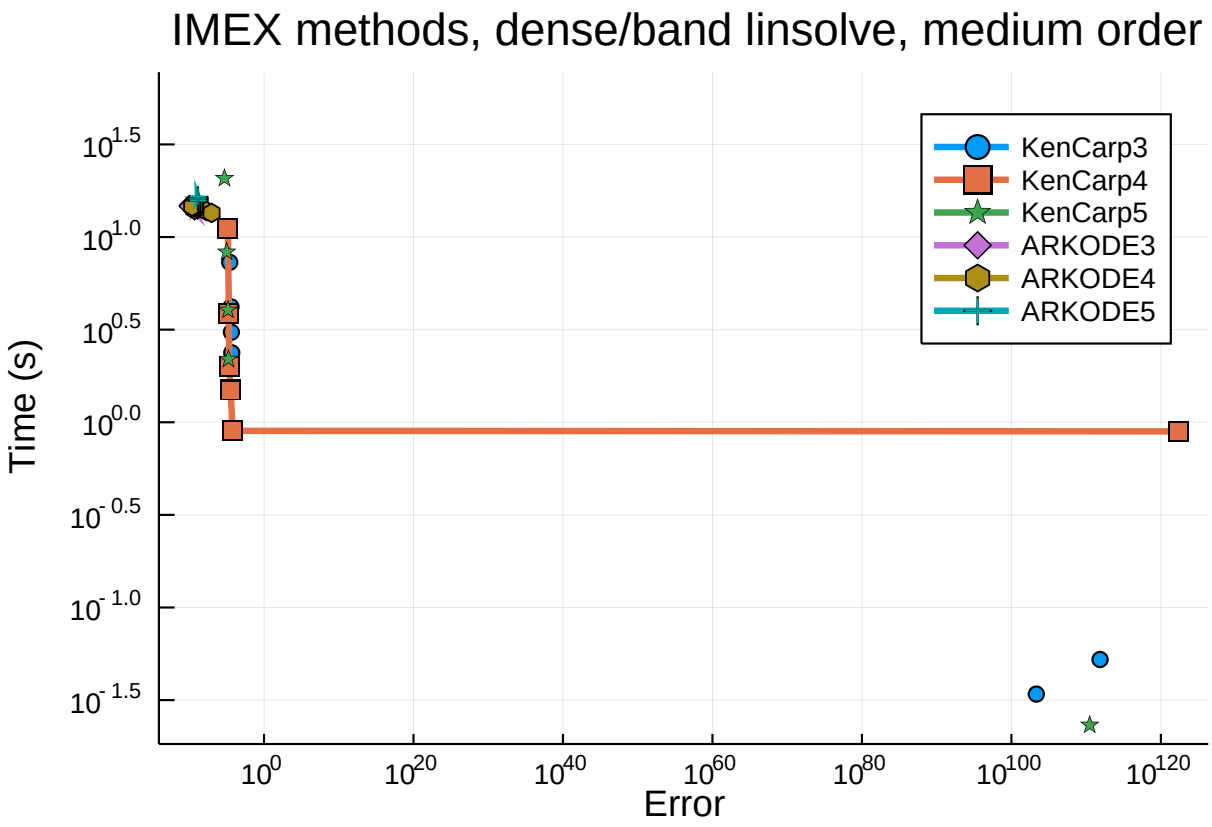
0.5 In-family comparisons

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));
```

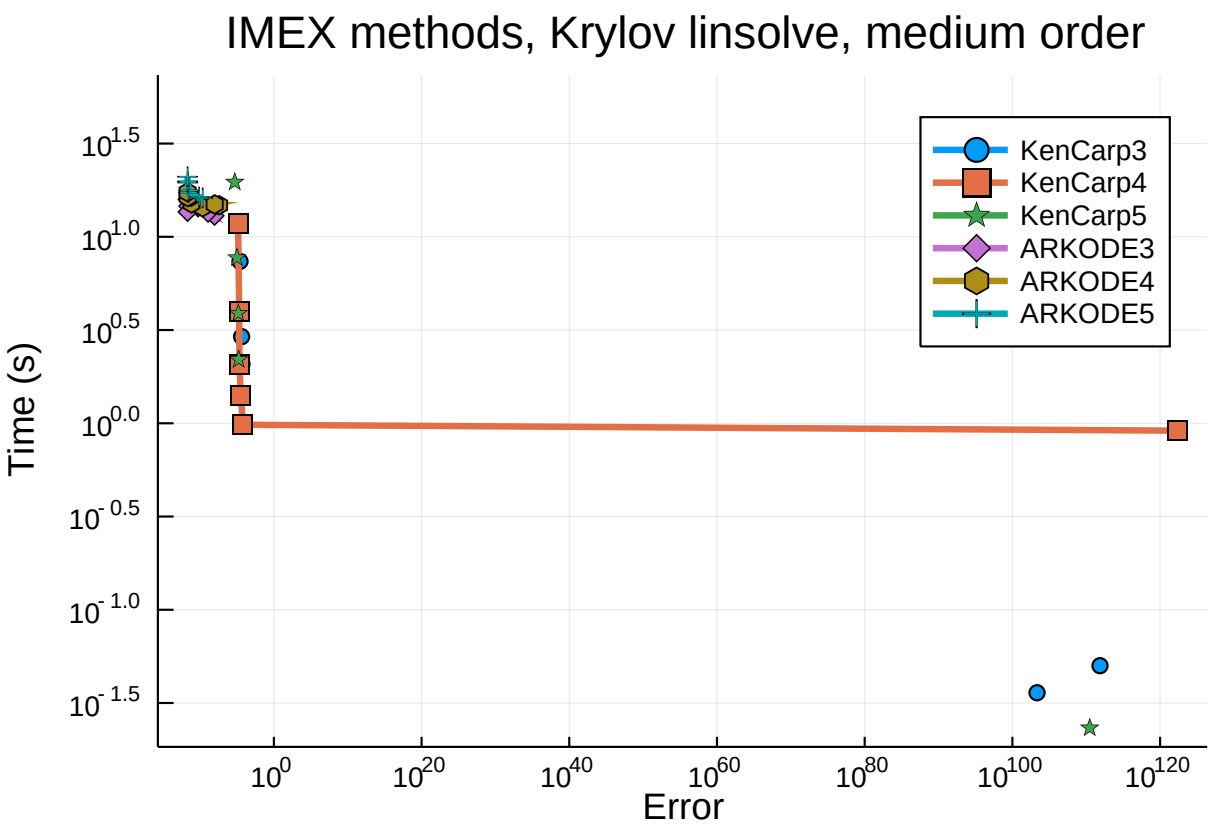
```
KenCarp3
KenCarp4
KenCarp5
ARKODE3
ARKODE4
ARKODE5
1372.092889 seconds (927.05 M allocations: 53.046 GiB, 2.30% gc time)
```

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



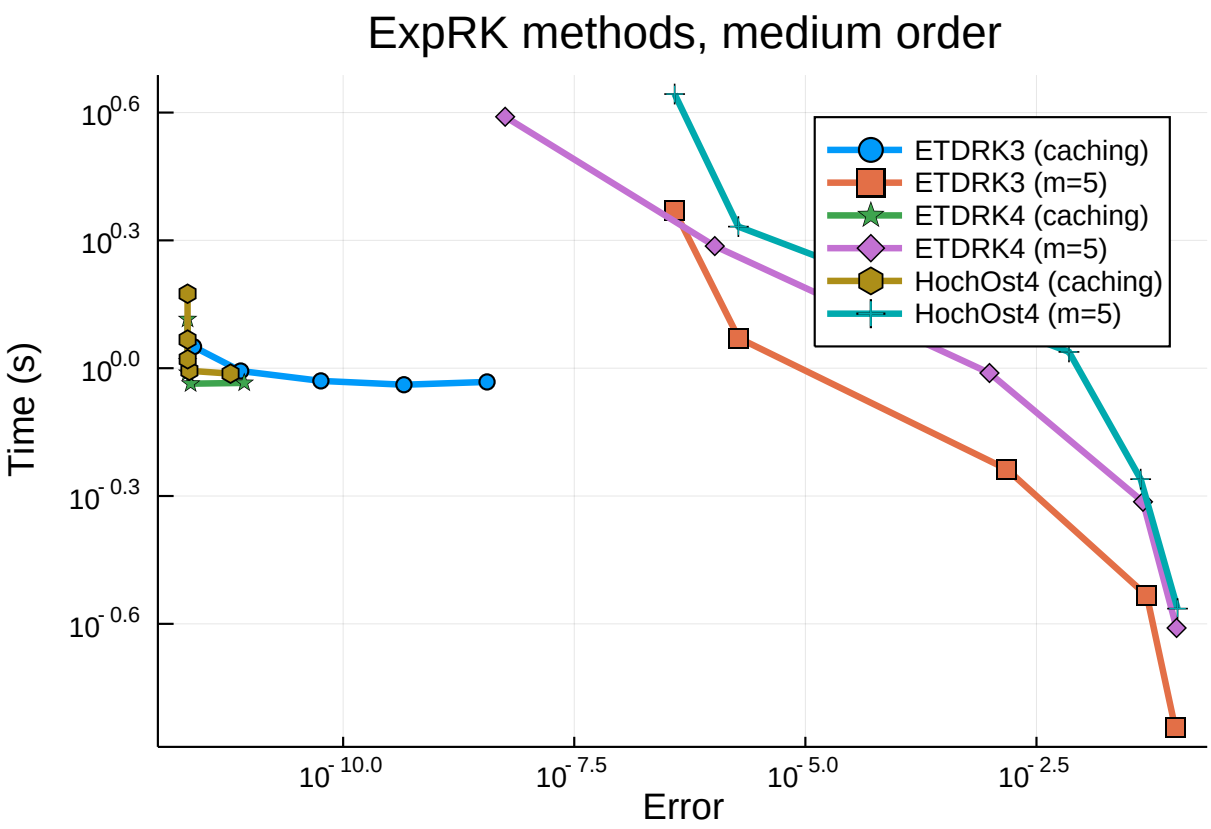
1.IMEX methods (krylov linear solver)

```
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
1441.475583 seconds (1.13 G allocations: 68.598 GiB, 2.59% gc time)

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



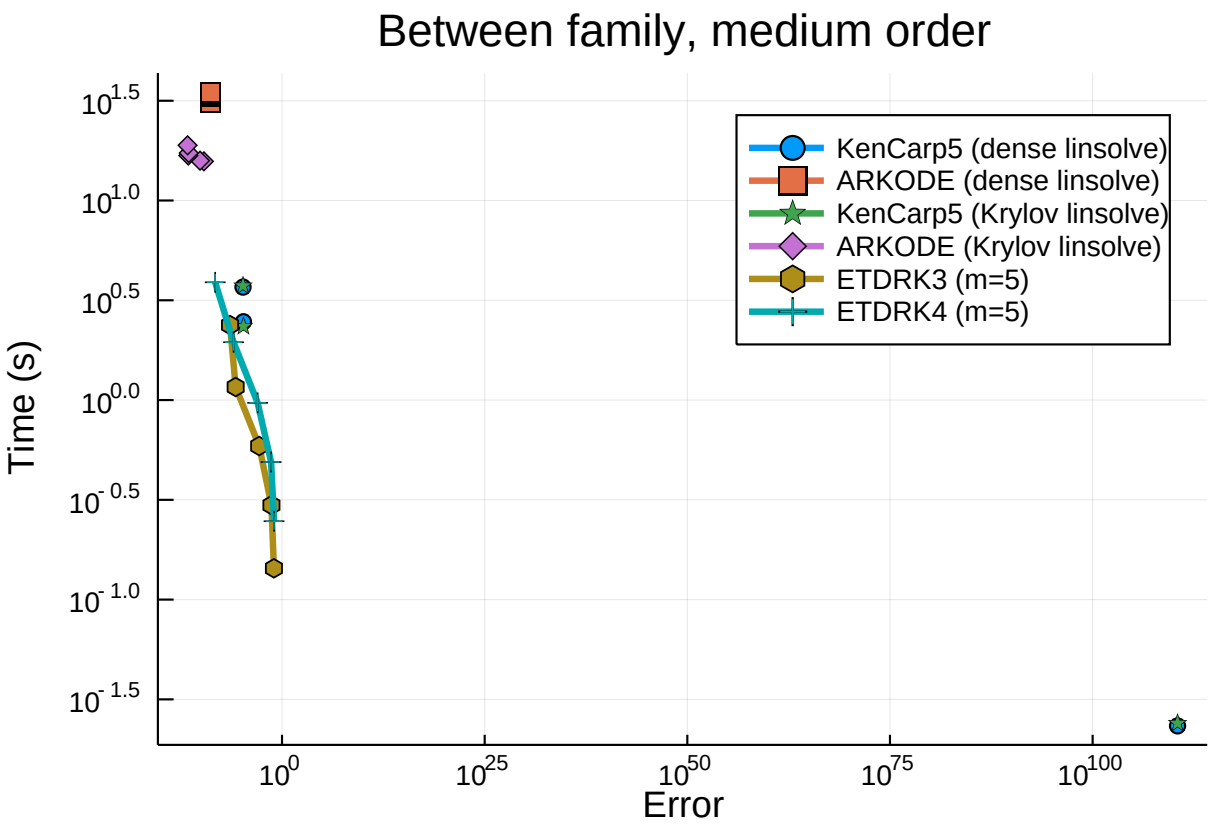
2.ExpRK methods

```
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)
222.282827 seconds (116.57 M allocations: 28.796 GiB, 6.58% 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)
857.334543 seconds (416.49 M allocations: 30.726 GiB, 1.89% 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 1.2.0
Commit c6da87ff4b (2019-08-20 00:03 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)
Environment:
  JULIA_NUM_THREADS = 16
```

Package Information:

```
Status: `/home/crackauckas/.julia/dev/DiffEqBenchmarks/Project.toml`
[28f2ccd6-bb30-5033-b560-165f7b14dc2f] ApproxFun 0.11.7
[a134a8b2-14d6-55f6-9291-3336d3ab0209] BlackBoxOptim 0.5.0
[eb300fae-53e8-50a0-950c-e21f52c2b7e0] DiffEqBiological 3.11.0
[f3b72e0c-5b89-59e1-b016-84e28bfd966d] DiffEqDevTools 2.15.0
[1130ab10-4a5a-5621-a13d-e4788d82bd4c] DiffEqParamEstim 1.8.0
[a077e3f3-b75c-5d7f-a0c6-6bc4c8ec64a9] DiffEqProblemLibrary 4.5.1
[ef61062a-5684-51dc-bb67-a0fcdec5c97d] DiffEqUncertainty 1.2.0
[7073ff75-c697-5162-941a-fcdaad2a7d2a] IJulia 1.20.0
[7f56f5a3-f504-529b-bc02-0b1fe5e64312] LSODA 0.6.1
[76087f3c-5699-56af-9a33-bf431cd00edd] NLopt 0.5.1
[c030b06c-0b6d-57c2-b091-7029874bd033] ODE 2.5.0
[54ca160b-1b9f-5127-a996-1867f4bc2a2c] ODEInterface 0.4.6
[09606e27-ecf5-54fc-bb29-004bd9f985bf] ODEInterfaceDiffEq 3.4.0
[1dea7af3-3e70-54e6-95c3-0bf5283fa5ed] OrdinaryDiffEq 5.17.2
[65888b18-ceab-5e60-b2b9-181511a3b968] ParameterizedFunctions 4.2.1
[91a5bcdd-55d7-5caf-9e0b-520d859cae80] Plots 0.26.3
[b4db0fb7-de2a-5028-82bf-5021f5cfa881] ReactionNetworkImporters 0.1.5
[f2c3362d-daeb-58d1-803e-2bc74f2840b4] RecursiveFactorization 0.1.0
[c3572dad-4567-51f8-b174-8c6c989267f4] Sundials 3.7.0
[44d3d7a6-8a23-5bf8-98c5-b353f8df5ec9] Weave 0.9.1
[b77e0a4c-d291-57a0-90e8-8db25a27a240] InteractiveUtils
[d6f4376e-aef5-505a-96c1-9c027394607a] Markdown
[44cfe95a-1eb2-52ea-b672-e2afdf69b78f] Pkg
[9a3f8284-a2c9-5f02-9a11-845980a1fd5c] Random
```