Negative Feedback Gene Expression Model

Samuel Isaacson, Chris Rackauckas

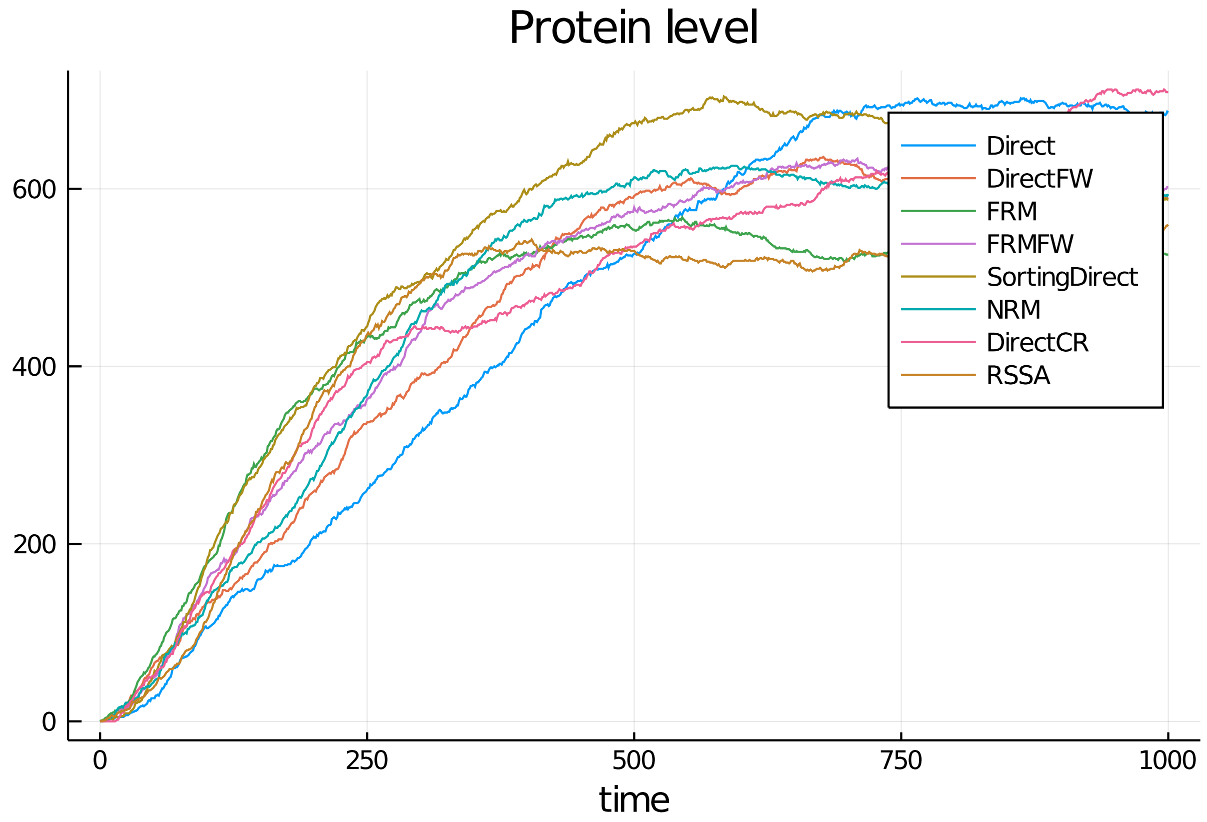
July 4, 2020

```
using DiffEqBase, DiffEqJump, DiffEqProblemLibrary, Plots, Statistics
using DiffEqProblemLibrary.JumpProblemLibrary: importjumpproblems; importjumpproblems()
import DiffEqProblemLibrary.JumpProblemLibrary: prob_jump_dnarepressor
gr()
fmt = :png
```

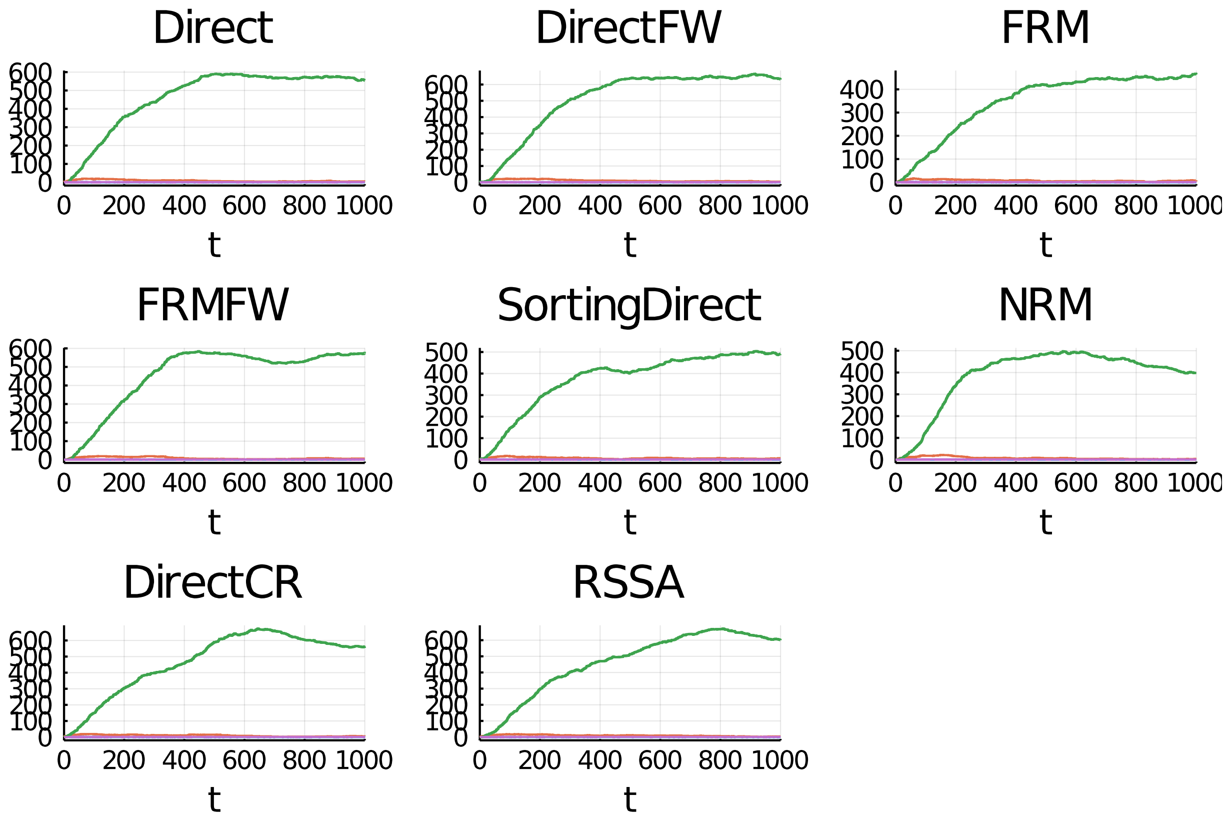
```
:png
```

1 Plot solutions by each method

```
methods = (Direct(),DirectFW(),FRM(),FRMFW(),SortingDirect(),NRM(),DirectCR(),RSSA())
shortlabels = [string(leg)[12:end-2] for leg in methods]
prob    = prob_jump_dnarepressor.discrete_prob
tf      = prob_jump_dnarepressor.tstop
rn      = prob_jump_dnarepressor.network
ploth   = plot(reuse=false)
for (i,method) in enumerate(methods)
    jump_prob = JumpProblem(prob, method, rn, save_positions=(false,false))
    sol = solve(jump_prob, SSAStepper(), saveat=tf/1000.)
    plot!(ploth,sol.t,sol[3,:],label=shortlabels[i], format=fmt)
end
plot(ploth, title="Protein level", xlabel="time",format=fmt)
```



```julia
p = []
for (i,method) in enumerate(methods)
    jump_prob = JumpProblem(prob, method, rn, save_positions=(false,false))
    sol = solve(jump_prob, SSAStepper(), saveat=tf/1000.)
    push!(p, plot(sol,title=shortlabels[i],leg=false,format=fmt))
end
plot(p...,format=fmt)
```

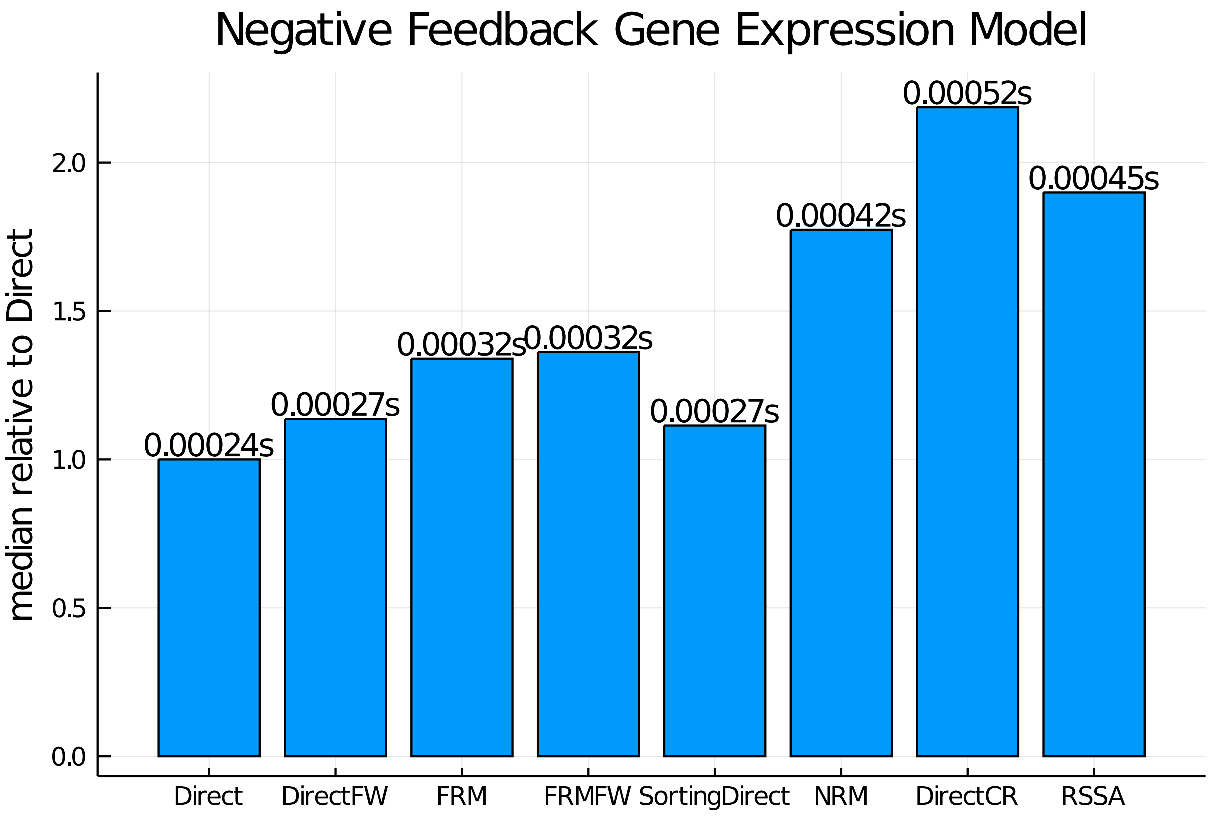


2 Benchmarking performance of the methods

```
function run_benchmark!(t, jump_prob, stepper)
    sol = solve(jump_prob, stepper)
    @inbounds for i in 1:length(t)
        t[i] = @elapsed (sol = solve(jump_prob, stepper))
    end
end

run_benchmark! (generic function with 1 method)

nsims = 500
benchmarks = Vector{Vector{Float64}}()
for method in methods
    jump_prob = JumpProblem(prob, method, rn, save_positions=(false,false))
    stepper = SSAStepper()
    t = Vector{Float64}(undef,nsims)
    run_benchmark!(t, jump_prob, stepper)
    push!(benchmarks, t)
end

medtimes = Vector{Float64}(undef,length(methods))
stdtimes = Vector{Float64}(undef,length(methods))
avgtimes = Vector{Float64}(undef,length(methods))
for i in 1:length(methods)
    medtimes[i] = median(benchmarks[i])
    avgtimes[i] = mean(benchmarks[i])
    stdtimes[i] = std(benchmarks[i])
end
println(medtimes/medtimes[1])
```

```
[1.0, 1.1367231282664818, 1.3394517557668493, 1.3613983166467267, 1.1142203
471653758, 1.773779988665701, 2.186291795227001, 1.8993304367902941]
```

```
using DataFrames
df =
DataFrame(names=shortlabels,medtimes=medtimes,relmedtimes=(medtimes/medtimes[1]),avgtimes=avgtimes,
std=stdtimes, cv=stdtimes./avgtimes)
sa = [text(string(round(mt,sigdigits=2),"s"),:center,10) for mt in df.medtimes]
bar(df.names,df.relmedtimes,legend=:false, fmt=fmt)
scatter!(df.names, .05 .+ df.relmedtimes, markeralpha=0, series_annotations=sa, fmt=fmt)
ylabel!("median relative to Direct")
title!("Negative Feedback Gene Expression Model")
```



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

2.1 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("Jumps","NegFeedback_GeneExpr.jmd")
```

Computer Information:

```
Julia Version 1.4.2
Commit 44fa15b150* (2020-05-23 18:35 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-8.0.1 (ORCJIT, skylake)
Environment:
  JULIA_DEPOT_PATH = /builds/JuliaGPU/DiffEqBenchmarks.jl/.julia
  JULIA_CUDA_MEMORY_LIMIT = 2147483648
  JULIA_PROJECT = @.
  JULIA_NUM_THREADS = 8
```

Package Information:

```
Status: `/builds/JuliaGPU/DiffEqBenchmarks.jl/benchmarks/Jumps/Project.toml`
[a93c6f00-e57d-5684-b7b6-d8193f3e46c0] DataFrames 0.21.4
[2b5f629d-d688-5b77-993f-72d75c75574e] DiffEqBase 6.40.4
[eb300fae-53e8-50a0-950c-e21f52c2b7e0] DiffEqBiological 4.3.0
[c894b116-72e5-5b58-be3c-e6d8d4ac2b12] DiffEqJump 6.9.3
[a077e3f3-b75c-5d7f-a0c6-6bc4c8ec64a9] DiffEqProblemLibrary 4.8.0
[1dea7af3-3e70-54e6-95c3-0bf5283fa5ed] OrdinaryDiffEq 5.41.0
[91a5bcdd-55d7-5caf-9e0b-520d859cae80] Plots 1.5.3
[10745b16-79ce-11e8-11f9-7d13ad32a3b2] Statistics
```