# Negative Feedback Gene Expression Model

### Samuel Isaacson, Chris Rackauckas

July 29, 2021

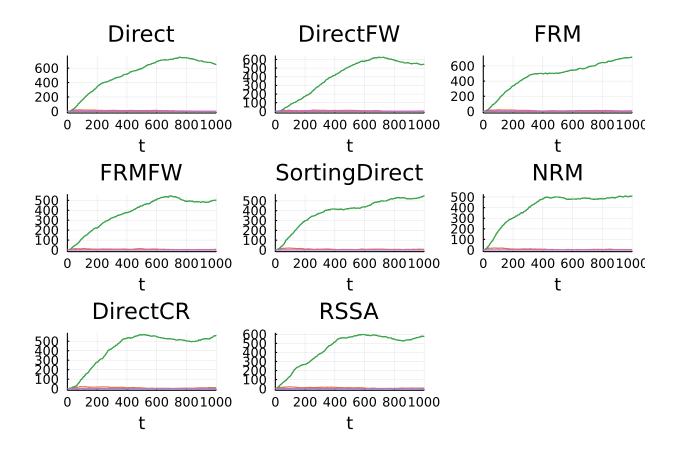
```
using DiffEqBase, DiffEqJump, DiffEqProblemLibrary, Plots, Statistics
using DiffEqProblemLibrary.JumpProblemLibrary: importjumpproblems; importjumpproblems()
import DiffEqProblemLibrary.JumpProblemLibrary: prob_jump_dnarepressor
gr()
fmt = :png
:png
```

## 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(rn, prob, method, 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)
```

## Protein level 800 Direct DirectFW FRM $\mathsf{FRMFW}$ SortingDirect 600 NRM DirectCR RSSA 400 200 0 250 500 1000 750 time

```
p = []
for (i,method) in enumerate(methods)
    jump_prob = JumpProblem(rn, prob, method, 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)
```



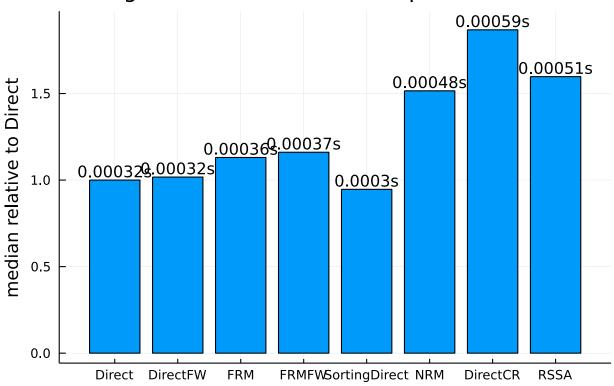
## 2 Benchmarking performance of the methods

```
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(rn, prob, method, 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, 1.017404500509805, 1.1305716927892253, 1.1608311795066355, 0.94644282 67691019, 1.5156822295465502, 1.8681020242018984, 1.5976303954346778]
```

```
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")
```





## 2.1 Appendix

These benchmarks are a part of the SciMLBenchmarks.jl repository, found at: https://github.com/SciML, For more information on high-performance scientific machine learning, check out the SciML Open Source Software Organization https://sciml.ai.

To locally run this benchmark, do the following commands:

```
using SciMLBenchmarks
SciMLBenchmarks.weave_file("benchmarks/Jumps","NegFeedback_GeneExpr.jmd")
```

Computer Information:

```
Julia Version 1.6.2
Commit 1b93d53fc4 (2021-07-14 15:36 UTC)
Platform Info:
```

```
OS: Linux (x86_64-pc-linux-gnu)
```

CPU: AMD EPYC 7502 32-Core Processor

WORD\_SIZE: 64 LIBM: libopenlibm

LLVM: libLLVM-11.0.1 (ORCJIT, znver2)

#### Environment:

JULIA\_DEPOT\_PATH = /root/.cache/julia-buildkite-plugin/depots/5b300254-1738-4989-ae0

### Package Information:

```
Status `/var/lib/buildkite-agent/builds/amdci3-julia-csail-mit-edu/julialang/scin[479239e8] Catalyst v6.13.0
[a93c6f00] DataFrames v1.1.1
[2b5f629d] DiffEqBase v6.62.2
[c894b116] DiffEqJump v6.14.2
[a077e3f3] DiffEqProblemLibrary v4.13.0
[961ee093] ModelingToolkit v5.19.1
[1dea7af3] OrdinaryDiffEq v5.57.0
[91a5bcdd] Plots v1.16.5
[31c91b34] SciMLBenchmarks v0.1.0
[10745b16] Statistics
```

### And the full manifest:

```
Status `/var/lib/buildkite-agent/builds/amdci3-julia-csail-mit-edu/julialang/sci
[c3fe647b] AbstractAlgebra v0.17.1
[1520ce14] AbstractTrees v0.3.4
[79e6a3ab] Adapt v3.3.1
[ec485272] ArnoldiMethod v0.1.0
[4fba245c] ArrayInterface v3.1.17
[4c555306] ArrayLayouts v0.7.0
[aae01518] BandedMatrices v0.16.9
[8e7c35d0] BlockArrays v0.15.3
[ffab5731] BlockBandedMatrices v0.10.6
[00ebfdb7] CSTParser v2.5.0
[479239e8] Catalyst v6.13.0
[d360d2e6] ChainRulesCore v0.9.45
[35d6a980] ColorSchemes v3.12.1
[3da002f7] ColorTypes v0.11.0
[5ae59095] Colors v0.12.8
[861a8166] Combinatorics v1.0.2
[a80b9123] CommonMark v0.8.1
[38540f10] CommonSolve v0.2.0
[bbf7d656] CommonSubexpressions v0.3.0
[34da2185] Compat v3.30.0
[b152e2b5] CompositeTypes v0.1.2
[8f4d0f93] Conda v1.5.2
```

```
[187b0558] ConstructionBase v1.2.1
```

[d38c429a] Contour v0.5.7

[a8cc5b0e] Crayons v4.0.4

[9a962f9c] DataAPI v1.6.0

[a93c6f00] DataFrames v1.1.1

[864edb3b] DataStructures v0.18.9

[e2d170a0] DataValueInterfaces v1.0.0

[2b5f629d] DiffEqBase v6.62.2

[c894b116] DiffEqJump v6.14.2

[9fdde737] DiffEqOperators v4.28.0

[a077e3f3] DiffEqProblemLibrary v4.13.0

[163ba53b] DiffResults v1.0.3

[b552c78f] DiffRules v1.0.2

[b4f34e82] Distances v0.10.3

[31c24e10] Distributions v0.24.18

[ffbed154] DocStringExtensions v0.8.5

[e30172f5] Documenter v0.26.3

[5b8099bc] DomainSets v0.5.2

[da5c29d0] EllipsisNotation v1.1.0

[d4d017d3] ExponentialUtilities v1.8.4

[e2ba6199] ExprTools v0.1.3

[c87230d0] FFMPEG v0.4.1

[7034ab61] FastBroadcast v0.1.8

[9aa1b823] FastClosures v0.3.2

[1a297f60] FillArrays v0.11.7

[6a86dc24] FiniteDiff v2.8.0

[53c48c17] FixedPointNumbers v0.8.4

[59287772] Formatting v0.4.2

[f6369f11] ForwardDiff v0.10.18

[069b7b12] FunctionWrappers v1.1.2

[28b8d3ca] GR v0.57.5

[5c1252a2] GeometryBasics v0.3.12

[d7ba0133] Git v1.2.1

[42e2da0e] Grisu v1.0.2

[cd3eb016] HTTP v0.9.10

[eafb193a] Highlights v0.4.5

[0e44f5e4] Hwloc v2.0.0

[7073ff75] IJulia v1.23.2

[b5f81e59] IOCapture v0.1.1

[615f187c] IfElse v0.1.0

[d25df0c9] Inflate v0.1.2

[83e8ac13] IniFile v0.5.0

[8197267c] IntervalSets v0.5.3

[41ab1584] InvertedIndices v1.0.0

[c8e1da08] IterTools v1.3.0

[42fd0dbc] IterativeSolvers v0.9.1

[82899510] IteratorInterfaceExtensions v1.0.0

[692b3bcd] JLLWrappers v1.3.0

[682c06a0] JSON v0.21.1

```
[98e50ef6] JuliaFormatter v0.13.7
```

- [b964fa9f] LaTeXStrings v1.2.1
- [2ee39098] LabelledArrays v1.6.1
- [23fbe1c1] Latexify v0.15.6
- [5078a376] LazyArrays v0.21.6
- [d7e5e226] LazyBandedMatrices v0.5.8
- [093fc24a] LightGraphs v1.3.5
- [d3d80556] LineSearches v7.1.1
- [2ab3a3ac] LogExpFunctions v0.2.4
- [bdcacae8] LoopVectorization v0.12.37
- [1914dd2f] MacroTools v0.5.6
- [a3b82374] MatrixFactorizations v0.8.3
- [739be429] MbedTLS v1.0.3
- [442fdcdd] Measures v0.3.1
- [e1d29d7a] Missings v1.0.0
- [961ee093] ModelingToolkit v5.19.1
- [46d2c3a1] MuladdMacro v0.2.2
- [ffc61752] Mustache v1.0.10
- [d41bc354] NLSolversBase v7.8.0
- [2774e3e8] NLsolve v4.5.1
- [872c559c] NNlib v0.7.21
- [77ba4419] NaNMath v0.3.5
- [8913a72c] NonlinearSolve v0.3.8
- [6fe1bfb0] OffsetArrays v1.9.2
- [bac558e1] OrderedCollections v1.4.1
- [1dea7af3] OrdinaryDiffEq v5.57.0
- [90014a1f] PDMats v0.11.1
- [d96e819e] Parameters v0.12.2
- [69de0a69] Parsers v1.1.0
- [ccf2f8ad] PlotThemes v2.0.1
- [995b91a9] PlotUtils v1.0.10
- [91a5bcdd] Plots v1.16.5
- [e409e4f3] PoissonRandom v0.4.0
- [f517fe37] Polyester v0.3.1
- [2dfb63ee] PooledArrays v1.2.1
- [21216c6a] Preferences v1.2.2
- [08abe8d2] PrettyTables v1.1.0
- [1fd47b50] QuadGK v2.4.1
- [fb686558] RandomExtensions v0.4.3
- [e6cf234a] RandomNumbers v1.4.0
- [3cdcf5f2] RecipesBase v1.1.1
- [01d81517] RecipesPipeline v0.3.2
- [731186ca] RecursiveArrayTools v2.11.4
- [f2c3362d] RecursiveFactorization v0.1.12
- [189a3867] Reexport v1.1.0
- [ae029012] Requires v1.1.3
- [79098fc4] Rmath v0.7.0
- [7e49a35a] RuntimeGeneratedFunctions v0.5.2
- [476501e8] SLEEFPirates v0.6.21

```
[1bc83da4] SafeTestsets v0.0.1
```

[Obca4576] SciMLBase v1.13.5

[31c91b34] SciMLBenchmarks v0.1.0

[6c6a2e73] Scratch v1.1.0

[efcf1570] Setfield v0.7.0

[992d4aef] Showoff v1.0.3

[699a6c99] SimpleTraits v0.9.3

[b85f4697] SoftGlobalScope v1.1.0

[a2af1166] SortingAlgorithms v1.0.0

[47a9eef4] SparseDiffTools v1.13.2

[276daf66] SpecialFunctions v1.5.1

[aedffcd0] Static v0.2.5

[90137ffa] StaticArrays v1.2.2

[82ae8749] StatsAPI v1.0.0

[2913bbd2] StatsBase v0.33.8

[4c63d2b9] StatsFuns v0.9.8

[7792a7ef] StrideArraysCore v0.1.13

[69024149] StringEncodings v0.3.4

[09ab397b] StructArrays v0.5.1

[d1185830] SymbolicUtils v0.11.3

[0c5d862f] Symbolics v0.1.32

[3783bdb8] TableTraits v1.0.1

[bd369af6] Tables v1.4.3

[8290d209] ThreadingUtilities v0.4.4

[a759f4b9] TimerOutputs v0.5.9

[0796e94c] Tokenize v0.5.16

[a2a6695c] TreeViews v0.3.0

[5c2747f8] URIs v1.3.0

[3a884ed6] UnPack v1.0.2

[1986cc42] Unitful v1.8.0

[3d5dd08c] VectorizationBase v0.20.16

[81def892] VersionParsing v1.2.0

[19fa3120] VertexSafeGraphs v0.1.2

[44d3d7a6] Weave v0.10.9

[ddb6d928] YAML v0.4.7

[c2297ded] ZMQ v1.2.1

[700de1a5] ZygoteRules v0.2.1

[6e34b625] Bzip2\_jll v1.0.6+5

[83423d85] Cairo jll v1.16.0+6

[5ae413db] EarCut\_jll v2.1.5+1

[2e619515] Expat jll v2.2.10+0

[b22a6f82] FFMPEG jll v4.3.1+4

[a3f928ae] Fontconfig\_jll v2.13.1+14

[d7e528f0] FreeType2\_jll v2.10.1+5

[559328eb] FriBidi\_jll v1.0.10+0

[0656b61e] GLFW jll v3.3.5+0

[d2c73de3] GR\_jll v0.57.3+0

[78b55507] Gettext\_jll v0.20.1+7

[f8c6e375] Git jll v2.31.0+0

```
[7746bdde] Glib jll v2.59.0+4
[e33a78d0] Hwloc jll v2.4.1+0
[aacddb02] JpegTurbo_jll v2.1.0+0
[c1c5ebd0] LAME jll v3.100.1+0
[dd4b983a] LZO jll v2.10.1+0
[dd192d2f] LibVPX_jll v1.10.0+0
[e9f186c6] Libffi jll v3.2.2+0
[d4300ac3] Libgcrypt jll v1.8.7+0
[7e76a0d4] Libglvnd jll v1.3.0+3
[7add5ba3] Libgpg_error_jll v1.42.0+0
[94ce4f54] Libiconv_jll v1.16.1+0
[4b2f31a3] Libmount_jll v2.35.0+0
[89763e89] Libtiff_jll v4.3.0+0
[38a345b3] Libuuid jll v2.36.0+0
[e7412a2a] Ogg jll v1.3.5+0
[458c3c95] OpenSSL jll v1.1.10+0
[efe28fd5] OpenSpecFun_jll v0.5.5+0
[91d4177d] Opus_jll v1.3.2+0
[2f80f16e] PCRE_jll v8.44.0+0
[30392449] Pixman jll v0.40.1+0
[ea2cea3b] Qt5Base jll v5.15.2+0
[f50d1b31] Rmath_jll v0.3.0+0
[a2964d1f] Wayland jll v1.17.0+4
[2381bf8a] Wayland_protocols_jll v1.18.0+4
[02c8fc9c] XML2_jll v2.9.12+0
[aed1982a] XSLT jll v1.1.34+0
[4f6342f7] Xorg libX11 jll v1.6.9+4
[OcOb7dd1] Xorg libXau jll v1.0.9+4
[935fb764] Xorg libXcursor jll v1.2.0+4
[a3789734] Xorg libXdmcp jll v1.1.3+4
[1082639a] Xorg_libXext_jll v1.3.4+4
[d091e8ba] Xorg libXfixes jll v5.0.3+4
[a51aa0fd] Xorg_libXi_jll v1.7.10+4
[d1454406] Xorg libXinerama jll v1.1.4+4
[ec84b674] Xorg libXrandr jll v1.5.2+4
[ea2f1a96] Xorg_libXrender_jll v0.9.10+4
[14d82f49] Xorg_libpthread_stubs_jll v0.1.0+3
[c7cfdc94] Xorg libxcb jll v1.13.0+3
[cc61e674] Xorg libxkbfile jll v1.1.0+4
[12413925] Xorg_xcb_util_image_jll v0.4.0+1
[2def613f] Xorg xcb util jll v0.4.0+1
[975044d2] Xorg xcb util keysyms jll v0.4.0+1
[Od47668e] Xorg_xcb_util_renderutil_jll v0.3.9+1
[c22f9ab0] Xorg_xcb_util_wm_jll v0.4.1+1
[35661453] Xorg xkbcomp jll v1.4.2+4
[33bec58e] Xorg xkeyboard config jll v2.27.0+4
[c5fb5394] Xorg_xtrans_jll v1.4.0+3
[8f1865be] ZeroMQ jll v4.3.2+6
[3161d3a3] Zstd jll v1.5.0+0
```

```
[0ac62f75] libass_jll v0.14.0+4
```

[f638f0a6] libfdk\_aac\_jll v0.1.6+4

[b53b4c65] libpng\_jll v1.6.38+0

[a9144af2] libsodium jll v1.0.20+0

[f27f6e37] libvorbis jll v1.3.7+0

[1270edf5] x264\_jll v2020.7.14+2

[dfaa095f] x265 jll v3.0.0+3

[d8fb68d0] xkbcommon\_jll v0.9.1+5

[Odad84c5] ArgTools

[56f22d72] Artifacts

[2a0f44e3] Base64

[ade2ca70] Dates

[8bb1440f] DelimitedFiles

[8ba89e20] Distributed

[f43a241f] Downloads

[7b1f6079] FileWatching

[9fa8497b] Future

[b77e0a4c] InteractiveUtils

[b27032c2] LibCURL

[76f85450] LibGit2

[8f399da3] Libdl

[37e2e46d] LinearAlgebra

[56ddb016] Logging

[d6f4376e] Markdown

[a63ad114] Mmap

[ca575930] NetworkOptions

[44cfe95a] Pkg

[de0858da] Printf

[3fa0cd96] REPL

[9a3f8284] Random

[ea8e919c] SHA

[9e88b42a] Serialization

[1a1011a3] SharedArrays

[6462fe0b] Sockets

[2f01184e] SparseArrays

[10745b16] Statistics

[4607b0f0] SuiteSparse

[fa267f1f] TOML

[a4e569a6] Tar

[8dfed614] Test

[cf7118a7] UUIDs

[4ec0a83e] Unicode

[e66e0078] CompilerSupportLibraries\_jll

[deac9b47] LibCURL\_jll

[29816b5a] LibSSH2\_jll

[c8ffd9c3] MbedTLS\_jll

[14a3606d] MozillaCACerts\_jll

[efcefdf7] PCRE2\_jll

[83775a58] Zlib jll

[8e850ede] nghttp2\_jll [3f19e933] p7zip\_jll