

# Diffusion Model

Samuel Isaacson, Chris Rackauckas

July 28, 2021

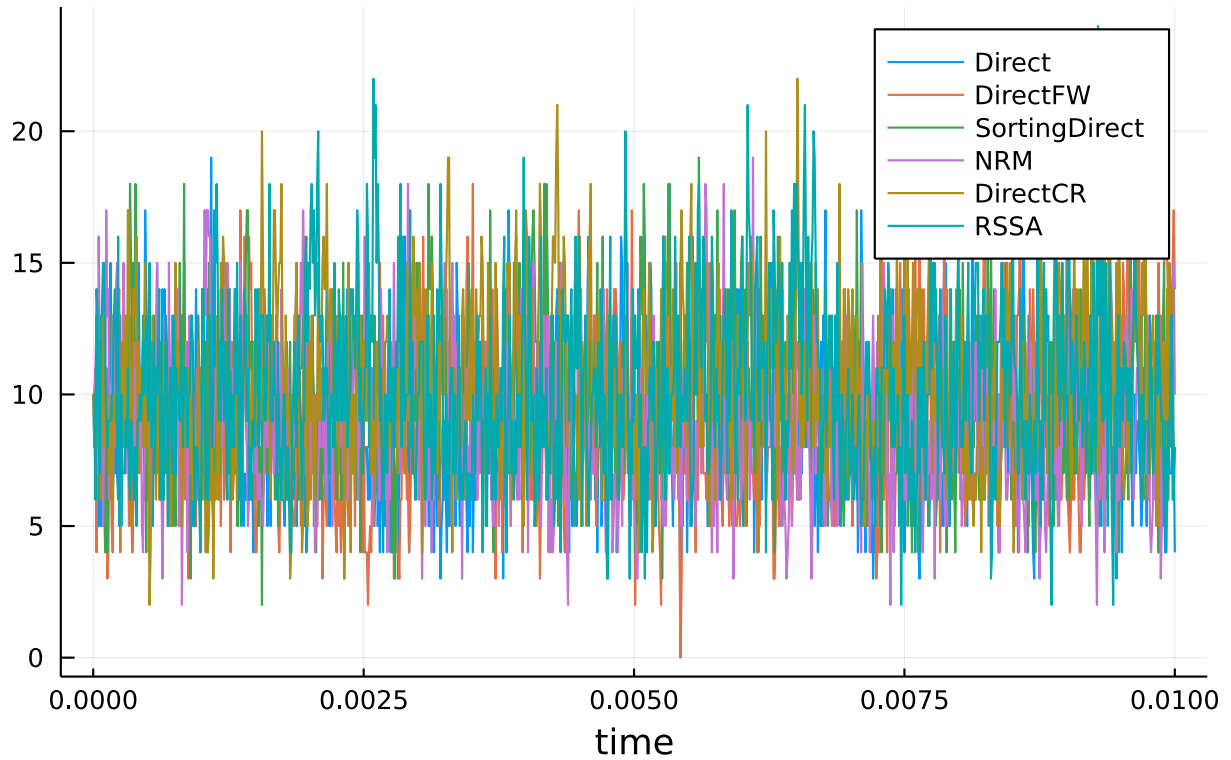
```
using DiffEqBase, Catalyst, DiffEqJump, DiffEqProblemLibrary.JumpProblemLibrary, Plots,  
Statistics, DataFrames  
gr()  
fmt = :png  
JumpProblemLibrary.importjumpproblems()
```

## 1 Model and example solutions

Here we implement a 1D continuous time random walk approximation of diffusion for  $N$  lattice sites on  $[0, 1]$ , with reflecting boundary conditions at  $x = 0$  and  $x = 1$ .

```
N = 256  
h = 1 / N  
u0 = 10*ones{Int64, N}  
tf = .01  
methods = (Direct(), DirectFW(), SortingDirect(), NRM(), DirectCR(), RSSA())  
shortlabels = [string(leg)[12:end-2] for leg in methods]  
jprob = prob_jump_diffnetwork  
prob = DiscreteProblem(u0, (0.0, tf), [1 / (h*h)])  
rn = jprob.network(N)  
ploth = plot(reuse=false)  
for (i, method) in enumerate(methods)  
    println("Benchmarking method: ", method)  
    jump_prob = JumpProblem(rn, prob, method, save_positions=(false, false))  
    sol = solve(jump_prob, SSAStepper(), saveat=tf/1000.)  
    plot!(ploth, sol.t, sol[Int(N//2),:], label=shortlabels[i], format=fmt)  
end  
plot!(ploth, title="Population at middle lattice site", xlabel="time", format=fmt)  
  
Benchmarking method: DiffEqJump.Direct()  
Benchmarking method: DiffEqJump.DirectFW()  
Benchmarking method: DiffEqJump.SortingDirect()  
Benchmarking method: DiffEqJump.NRM()  
Benchmarking method: DiffEqJump.DirectCR()  
Benchmarking method: DiffEqJump.RSSA()
```

## Population at middle lattice site



## 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 = 50
benchmarks = Vector{Vector{Float64}}{ }
for method in methods
    jump_prob = JumpProblem(rn, prob, method, save_positions=(false, false))
    stepper = SSAS stepper()
    t = Vector{Float64}(undef, nsims)
    run_benchmark!(t, jump_prob, stepper)
    push!(benchmarks, t)
end

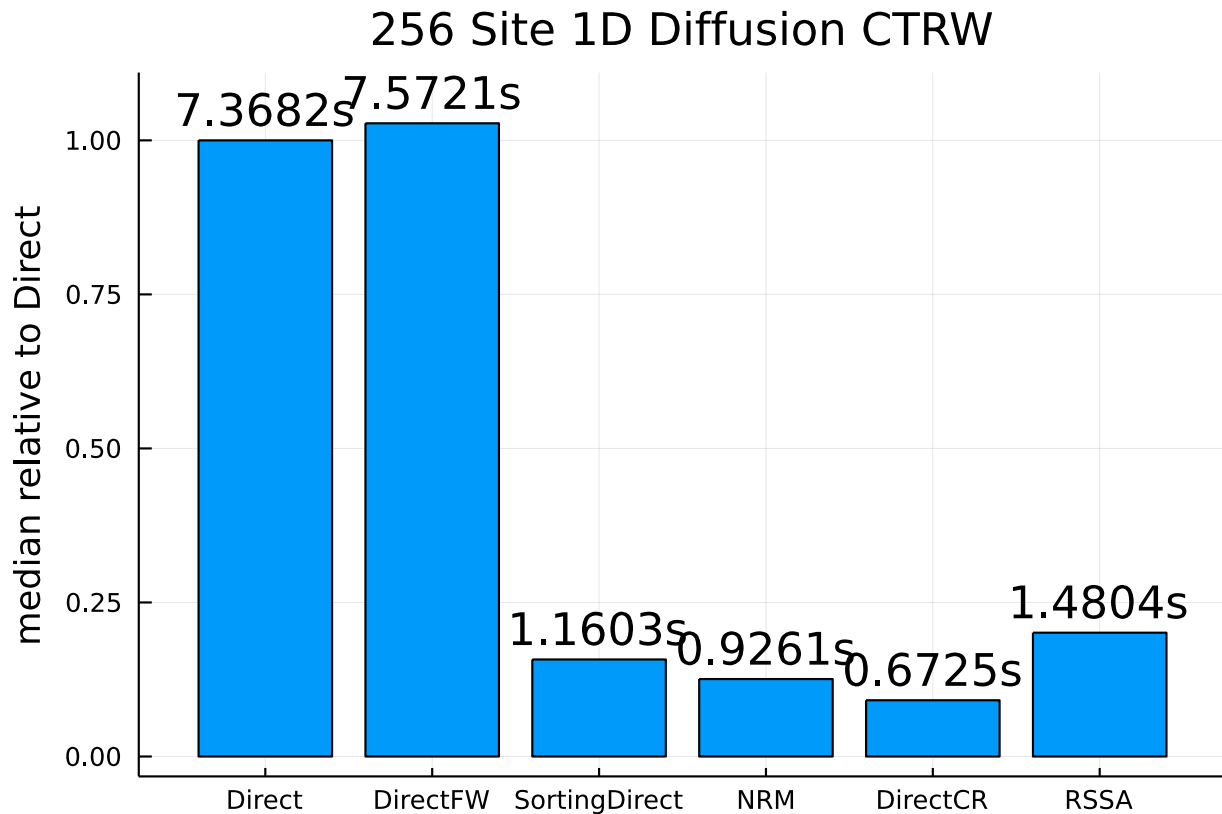
medtimes = Vector{Float64}(undef, length(methods))
stdtimes = Vector{Float64}(undef, length(methods))
avgtimes = Vector{Float64}(undef, length(methods))
for i in 1:length(methods)
    medtimes[i] = median(benchmarks[i])
    avgtimes[i] = mean(benchmarks[i])
    stdtimes[i] = std(benchmarks[i])
end
```

```
df = DataFrame(names=shortlabels, medtimes=medtimes, relmedtimes=(medtimes/medtimes[1]),
               avgtimes=avgtimes, std=stdtimes, cv=stdtimes./avgtimes)
```

	names	medtimes	relmedtimes	avgtimes	std	cv
	String	Float64	Float64	Float64	Float64	Float64
1	Direct	7.36819	1.0	7.36767	0.0147288	0.00199911
2	DirectFW	7.57214	1.02768	7.57204	0.00842374	0.00111248
3	SortingDirect	1.1603	0.157474	1.15989	0.00418625	0.00360916
4	NRM	0.926051	0.125682	0.927213	0.00508959	0.00548912
5	DirectCR	0.672495	0.0912701	0.674271	0.0094952	0.0140822
6	RSSA	1.48039	0.200917	1.48031	0.00255837	0.00172826

### 3 Plotting

```
sa = [string(round(mt,digits=4),"s") 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!("256 Site 1D Diffusion CTRW")
```



#### 3.1 Appendix

These benchmarks are a part of the SciMLBenchmarks.jl repository, found at: <https://github.com/SciML/SciMLBenchmarks.jl>. 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", "Diffusion_CTRW.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/sci
[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] SLEEF Pirates v0.6.21  
[1bc83da4] SafeTestsets v0.0.1  
[0bca4576] 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] LZ0\_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  
[0c0b7dd1] 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



[0d47668e] 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  
[0dad84c5] 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  
[efcefd7] PCRE2\_jll  
[83775a58] Zlib\_jll  
[8e850ede] nghttp2\_jll  
[3f19e933] p7zip\_jll