[1]:
```
using Markdown
```

[2]:
```
using LaTeXStrings, DifferentialEquations, LinearAlgebra,␣
↪Plots, SparseArrays
```

[3]:
```
using ForwardDiff
```

1 Self Activating Toggle Switch

Add required function to implement model

[4]:
```
begin
        mma(x) = 1/(1+x)
        mmr(x) = 1/(1+1/x)
        hfr(n) = x -> 1/(1 + x^n)
        hfa(n) = x -> 1/(1 + (1/x)^n)
        hs( , n) = x-> hfr(n)(x) +   * hfa(n)(x)
        hs( , n, x ) = x-> hs( , n)(x/x )
end
```

[4]:
```
hs (generic function with 2 methods)
```

Implement model piecewise (separate production and degradation terms) for simulations and computation

[5]:
```
begin
        n = 4 # hill coefficient
          = 3 # for bistable
          = 10 # for tristable
          = 0.1 # repressor
        x  = 80 # cutoff count bistable
        x  = 25 # cutoff count tristable
        x  = 20 # cuttoff count repress
        p = 5 # unregulated production rate
        d = 0.1 # death rate
        proda(a,b) = p*hs( , n, x )(a)*hs( , n, x )(b)
        dega(a, b) = d*a
        dadt(a, b) = proda(a, b) - dega(a, b)
        prodb(a, b) = proda(b, a)
        degb(a, b)= d*b
```

```
        dbdt(a, b) = prodb(a,b) - degb(a, b)
        dfx = dadt
        dfy = dbdt
end
```

[5]: dbdt (generic function with 1 method)

[6]:
```
begin
        fx(x::Vector) = dfx(x[1], x[2])
    fy(x::Vector) = dfy(x[1], x[2])
    f(x::Vector) = [fx(x), fy(x)]
end
```

[6]: f (generic function with 1 method)

Run Helmholtz decomposition using ForwardDiff for the divergence

[7]:
```
begin
        # savefig(p_pot, "ch4_comp_pot.pdf")
        # savefig(p_rhs, "ch4_comp_rhs.pdf")
end
```

Compute Vector Field

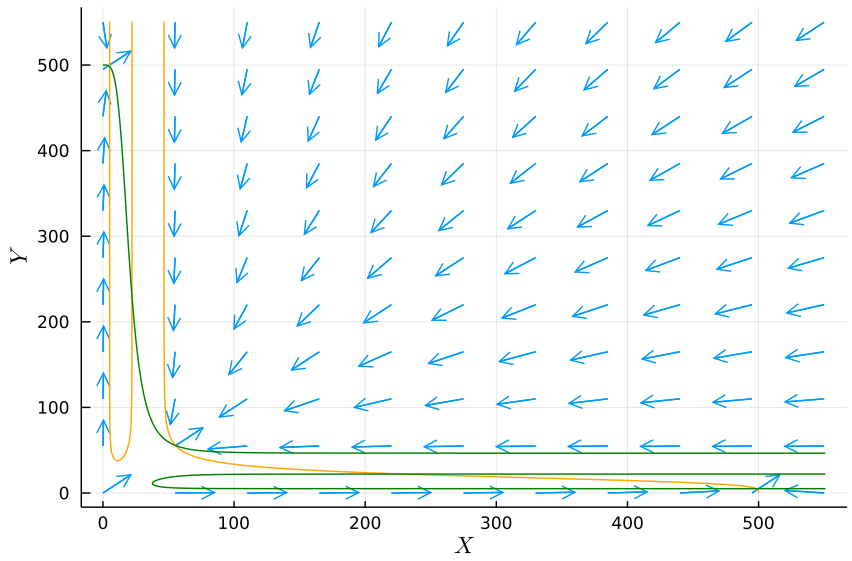
[8]:
```
begin
        n_min = 0
        n_max = 550
end
```

[8]: 550

[9]:
```
begin
        dq = (n_max - n_min) / 10.
        xs = n_min:dq:n_max+1
        ys = n_min:dq:n_max+1

        dxs = n_min:.5:n_max+1
        dys = n_min:.5:n_max+1

        df(x, y) = normalize([dfx(x, y), dfy(x,y)]) .* 30
```

```
        xxs = [x for x in xs for y in ys]
        yys = [y for x in xs for y in ys]

        quiver(xxs, yys, quiver=df)
        contour!(dxs, dys, dfx, levels=[0], color=:orange,␣
↪label="X Nullcline", colorbar = false)
        contour!(dxs, dys, dfy, levels=[0], color=:green,␣
↪label = "Y Nullcline", colorbar = false, xlabel=L"X",␣
↪ylabel=L"Y", legend=:topright,)
end
```

[9]:



[10]:

```
begin
        random_count() = floor(Int, n_min + rand() * (n_max␣
↪- n_min))
        rand_u0() = [random_count(), random_count()]
        u0 = rand_u0()
        u0 = [5, 500]
        t = (0.0, 30000.0)
end
```

[10]: (0.0, 30000.0)

Stochastic DiffEq of Langevin equation for this system

[11]:
```
begin
        function f(du, u, p, t)
                du[1] = dfx(u...)
                du[2] = dfy(u...)
                du[1], du[2]
        end

        g(du, u, p, t) = begin
          du[1,1] = sqrt(abs(proda(u[1], u[2])))
          du[1,2] = -sqrt(abs(degb(u[1], u[2])))
          du[1,3] = 0
          du[1,4] = 0
          du[2,1] = 0
          du[2,2] = 0
          du[2,3] = sqrt(abs(prodb(u[1], u[2])))
          du[2,4] = -sqrt(abs(degb(u[1], u[2])))
        end
end
```

[11]: g (generic function with 1 method)

[12]:
```
begin

        minval = 1
        maxval =  505
        nsample = 256
        rhs_xs = range(minval, maxval, length=nsample)
        rhs_ys = range(minval, maxval, length=nsample)

        divergence(F::Function, pt) = sum(
            diag(
                ForwardDiff.jacobian(F, pt)
                )
            )
```

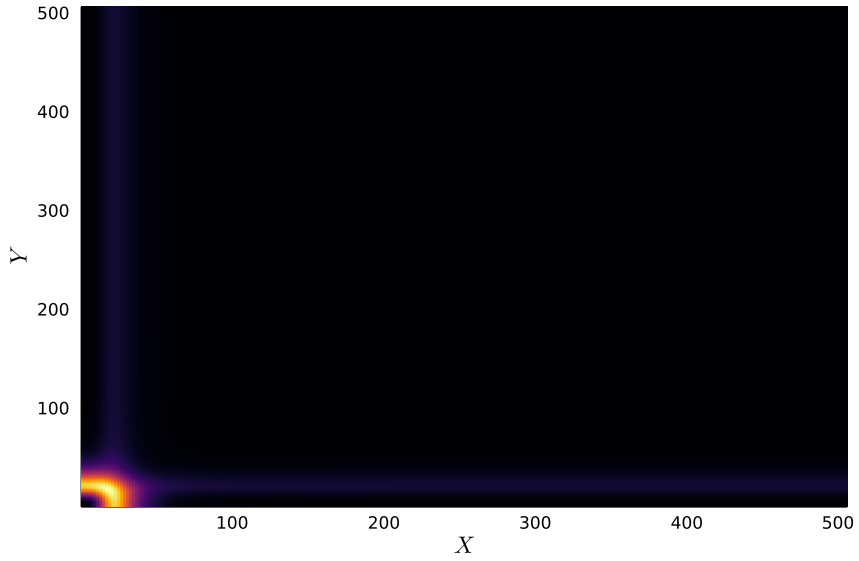
```
        rhs_new = [divergence(f, [x, y]) for x=rhs_xs,␣
↪y=rhs_ys]
end
```

[12]:
```
256×256 Matrix{Float64}:
 -0.199078  -0.187393   -0.143724    -0.048019    …  -0.
↪199952    -0.199952
 -0.187393  -0.175718   -0.132103    -0.0365489      -0.
↪198783    -0.198783
 -0.143724  -0.132103   -0.0887429    0.00611913     -0.
↪194416    -0.194416
 -0.048019  -0.0365489   0.00611913   0.0991794      -0.
↪184845    -0.184845
  0.115702   0.126852    0.168112     0.257596       -0.
↪168471    -0.168471
  0.353829   0.364426    0.403307     0.486866    …  -0.
↪144656    -0.144656
  0.656163   0.66594     0.701367     0.776451       -0.
↪114419    -0.11442
  0.991237   0.99996     1.03101      1.09549        -0.
↪0809077   -0.0809078
  1.30949    1.31701     1.34317      1.39599        -0.
↪0490778   -0.0490779
  1.55691    1.56323     1.58454      1.62601        -0.
↪0243302   -0.0243303
  1.69413    1.69934     1.71634      1.74792    …  -0.
↪0106041   -0.0106042
  1.70966    1.71394     1.72742      1.75126        -0.
↪00904762  -0.00904771
  1.61978    1.62331     1.63414      1.65243        -0.
↪0180329   -0.0180329
                                                      ␣
↪
 -0.199951  -0.198783   -0.194416    -0.184844       -0.2   ␣
↪      -0.2
 -0.199951  -0.198783   -0.194416    -0.184844    …  -0.2   ␣
↪      -0.2
```

```
-0.199951  -0.198783   -0.194416    -0.184844       -0.2   ␣
↪     -0.2
-0.199951  -0.198783   -0.194416    -0.184844       -0.2   ␣
↪     -0.2
-0.199951  -0.198783   -0.194416    -0.184845       -0.2   ␣
↪     -0.2
-0.199952  -0.198783   -0.194416    -0.184845       -0.2   ␣
↪     -0.2
-0.199952  -0.198783   -0.194416    -0.184845    …  -0.2   ␣
↪     -0.2
-0.199952  -0.198783   -0.194416    -0.184845       -0.2   ␣
↪     -0.2
-0.199952  -0.198783   -0.194416    -0.184845       -0.2   ␣
↪     -0.2
-0.199952  -0.198783   -0.194416    -0.184845       -0.2   ␣
↪     -0.2
-0.199952  -0.198783   -0.194416    -0.184845       -0.2   ␣
↪     -0.2
-0.199952  -0.198783   -0.194416    -0.184845    …  -0.2   ␣
↪     -0.2
```

[13]:
```
begin
        p_rhs = heatmap(rhs_xs, rhs_ys, rhs_new,␣
 ↪xlabel=L"X", ylabel=L"Y", colorbar=:none)
end
```

[13]:



[14]:
```
begin
        sde_prob_ssa= SDEProblem(f, g, u0, t,␣
 ↪noise_rate_prototype=zeros(2,4))
        sde_sol = solve(sde_prob_ssa)
end
```

```
 Warning: dt <= dtmin. Aborting. There is either an error in␣
 ↪your model
specification or the true solution is unstable.
  @ SciMLBase
/Users/bsm/.julia/packages/SciMLBase/EFFG1/src/
 ↪integrator_interface.jl:345
```

[14]:
```
retcode: DtLessThanMin
Interpolation: 1st order linear
t: 86999-element Vector{Float64}:
     0.0
     2.910508956835909e-7
     6.184831533276307e-7
     9.868444431771756e-7
```

```
    1.4012508942579135e-6
    1.8674581517237437e-6
    2.3919413163728028e-6
    2.981984876602994e-6
    3.6457838818619595e-6
    4.392557762778295e-6
    5.232678378809173e-6
    6.177814071843911e-6
    7.241091726507992e-6

 23542.178575796537
 23542.360200730658
 23542.564528781546
 23542.794397838796
 23543.0530005282
 23543.32353513031
 23543.62385721609
 23543.941567437698
 23544.298991437005
 23544.701093436222
 23545.036843327278
 23545.12194082928
u: 86999-element Vector{Vector{Float64}}:
 [5.0, 500.0]
 [4.998445499790408, 499.99895879479806]
 [4.997974996095271, 500.00155249337115]
 [4.993974986150907, 499.9925236185461]
 [4.99456314914844, 499.98940826985404]
 [4.987631615670938, 499.98308519113345]
 [4.979020646960344, 499.988146432747]
 [4.979027603686411, 499.9933952524822]
 [4.983127921293282, 500.00367991927766]
 [4.9852627746511535, 499.9891290717687]
 [4.978592030023531, 499.9830865840751]
 [4.990949022250143, 499.97542770348434]
 [4.9873859164715775, 499.9880802729246]

 [509.6778883567199, 2.515676347317035]
 [507.92930830626113, 2.2390995128380506]
```

```
 [513.1970347842835, 2.6736502613242403]
 [514.0679974631289, 1.980974826003427]
 [513.9293820330126, 1.4510163072278337]
 [506.6417203506271, 1.1809938031997163]
 [505.4938321605557, 0.7786902100306531]
 [508.8772868291129, 0.8460896694666321]
 [503.7106289597263, 0.7714335774043232]
 [500.3387980805558, 0.8522335110572933]
 [494.907105494683, 0.4419863327350493]
 [494.99057935601473, 0.2933383726336846]
```

[15]:
```
sde_plot = plot(sde_sol, vars=[(1, 2)], xlabel=L"X",␣
↪ylabel=L"Y",legend=:none)
savefig(sde_plot, "SATS_sde_plot.pdf")
```

Gillespie Jump Process formulation for the same problem

[16]:
```
begin
        proda!(integrator) = integrator.u[1] += 1
        prodb!(integrator) = integrator.u[2] += 1
        dega!(integrator) = integrator.u[1] -= 1
        degb!(integrator) = integrator.u[2] -= 1
        jumps = Dict(proda => proda!, prodb => prodb!, dega␣
↪=> dega!, degb => degb!)
        constJumps = []
        for (rate, jump) in jumps
                push!(constJumps, ConstantRateJump((u, p, t)␣
↪-> rate(u...), jump))
        end
        constJumps
end
```

[16]:
```
4-element Vector{Any}:
 ConstantRateJump{var"#17#18"{typeof(proda)},
typeof(proda!)}(var"#17#18"{typeof(proda)}(proda), proda!)
 ConstantRateJump{var"#17#18"{typeof(prodb)},
typeof(prodb!)}(var"#17#18"{typeof(prodb)}(prodb), prodb!)
 ConstantRateJump{var"#17#18"{typeof(degb)},
typeof(degb!)}(var"#17#18"{typeof(degb)}(degb), degb!)
```

```
 ConstantRateJump{var"#17#18"{typeof(dega)},
typeof(dega!)}(var"#17#18"{typeof(dega)}(dega), dega!)
```

[17]:
```
begin
        dprob_ssa = DiscreteProblem(u0, t)
        jprob_ssa = JumpProblem(dprob_ssa, Direct(),␣
 ↪constJumps...)
end
```

[17]:
```
Number of constant rate jumps: 4
Number of variable rate jumps: 0
```

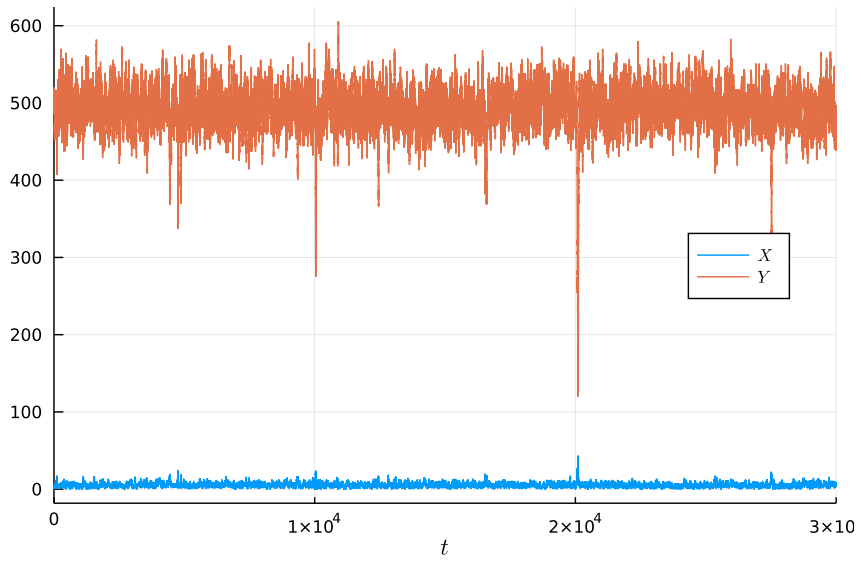
[18]:
```
ssa_sol = solve(jprob_ssa, SSAStepper())
```

[18]:
```
retcode: Default
Interpolation: Piecewise constant interpolation
t: 2988833-element Vector{Float64}:
     0.0
     0.024071853846978065
     0.0327441707559156
     0.04583388690915828
     0.053568418325886526
     0.05794376413794675
     0.06908809325132233
     0.06921299584568397
     0.0960160332234628
     0.11683317974055703
     0.11790643564601012
     0.12368853279393327
     0.1275023979197143

 29999.808281144095
 29999.809659479415
 29999.81150217346
 29999.836692508652
 29999.84321426462
 29999.85148324632
```

```
 29999.866360965807
 29999.889562441207
 29999.933240361588
 29999.986323294124
 29999.997285986006
 30000.0
u: 2988833-element Vector{Vector{Int64}}:
 [5, 500]
 [5, 501]
 [5, 500]
 [5, 499]
 [5, 498]
 [5, 499]
 [5, 498]
 [5, 499]
 [5, 500]
 [5, 501]
 [5, 500]
 [5, 501]
 [5, 502]

 [6, 488]
 [6, 489]
 [6, 488]
 [6, 487]
 [6, 488]
 [6, 489]
 [6, 490]
 [6, 489]
 [6, 488]
 [6, 487]
 [6, 486]
 [6, 486]
```

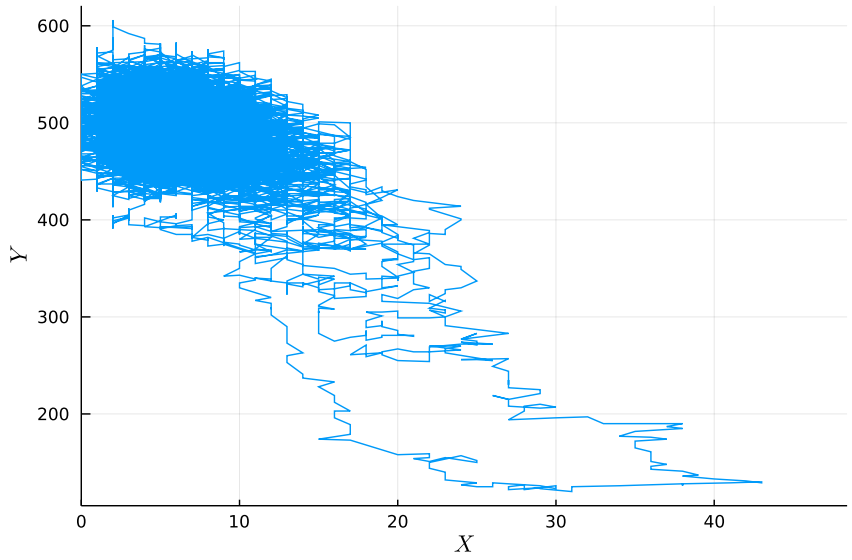
[19]:
```
stoch_tri = plot(ssa_sol, labels=[L"X" L"Y"], xlabel=L"t",␣
↪legend=(0.9, 0.5))
```

[19]:



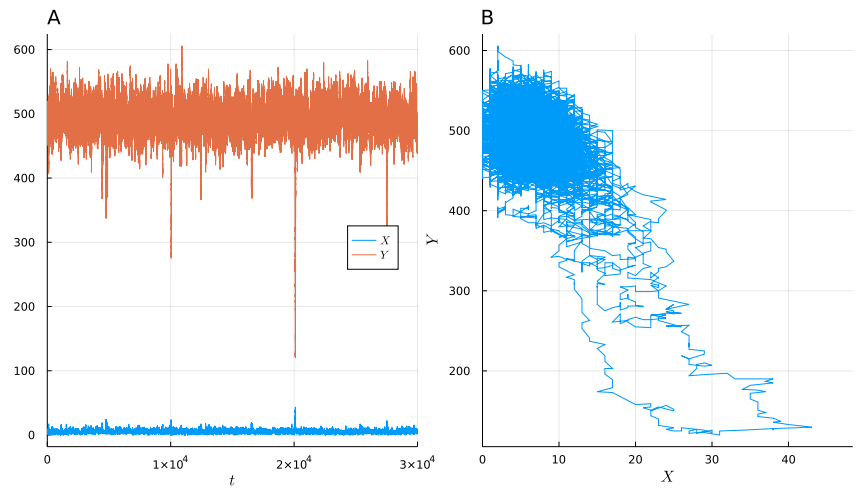
[20]:
```
stoch_tri3 = plot(ssa_sol, vars=[(1, 2)], xlabel=L"X",␣
↪ylabel=L"Y",legend=:none)
```

[20]:



[21]:
```
pstoch = plot(stoch_tri, stoch_tri3, layout=(1, 2),␣
 ↪size=(900, 500), title = ["A" "B"], titlelocation = :left)
```

[21]:



[22]:
```
# savefig(pstoch, "ch4_tri_stoch.pdf")
```

Setup helper functions for running longer simulations

[23]:
```
function get_u0(i)
        offset = 1.0
        new_u0 = [0.0, 0.0]
        if i % 3 == 0
                new_u0 = [55, 55]
        elseif i % 3 == 1
                new_u0 .+= [5, 500]
        elseif i % 3 == 2
                new_u0 .+= [500, 5]
        end
        new_u0
end
```

[23]:
```
get_u0 (generic function with 1 method)
```

[24]:
```
# savefig(ps, "ch4_ad_hoc.pdf")
```

Helper function to generate - ^{2} to solve the Helmhotz equation

[25]:
```
begin
        eye(N, M) = sparse(I, N, M)
        eye(M) = eye(M, M)
        diff1(M) = [ [1.0 zeros(1, M - 1)]; diagm(1 =>␣
↪ones(M - 1)) - eye(M) ]
        sdiff1(M) = sparse(diff1(M))

        # make the discrete -Laplacian in 2d, with Dirichlet␣
↪boundaries
        function laplacian2d(Nx, Ny, Lx, Ly)
                dx = Lx / (Nx + 1)
                dy = Ly / (Ny + 1)
                Dx = sdiff1(Nx) / dx
                Dy = sdiff1(Ny) / dy
                Ax = Dx' * Dx
                Ay = Dy' * Dy
                return Dx, Dy, kron(eye(Ny), Ax) + kron(Ay,␣
↪eye(Nx))
        end
end
```

[25]:
```
laplacian2d (generic function with 1 method)
```

[26]:
```
begin
        _, _, Δ = laplacian2d(nsample, nsample, maxval -␣
↪minval, maxval - minval)
        sol = reshape(Δ \ reshape(rhs_new, length(rhs_new)),␣
↪ size(rhs_new)...)
end
```

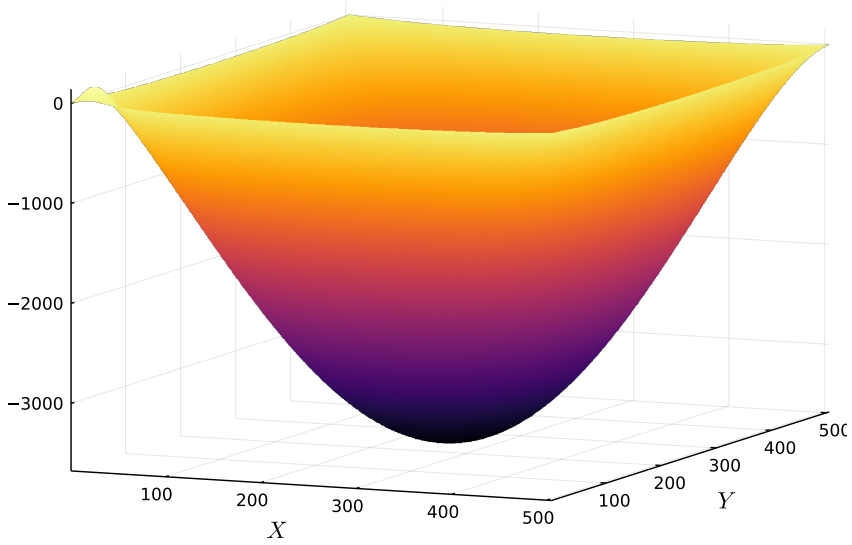
[26]:
```
256×256 Matrix{Float64}:
   2.43212    5.24705    8.33599  …   -5.38033   -3.85295  ␣
↪-2.11273
   5.24705   10.9408    16.9724      -10.1287    -7.14974  ␣
↪-3.829
```

```
  8.33599   16.9724    25.8132      -14.3517   -10.0239   ␣
↪-5.28902
 11.6773    23.3077    34.8246      -18.1302   -12.5573   ␣
↪-6.55551
 15.25      29.897     43.9402      -21.5325   -14.8086   ␣
↪-7.66486
 18.9807    36.6024    52.9804   …  -24.6278   -16.8317   ␣
↪-8.64743
 22.7098    43.1499    61.6013      -27.4953   -18.6869   ␣
↪-9.5368
 26.1849    49.125     69.2949      -30.2262   -20.4437   ␣
↪-10.3728
 29.0928    54.0244    75.4539      -32.9186   -22.1777   ␣
↪-11.1996
 31.1257    57.3611    79.4972      -35.6641   -23.9601   ␣
↪-12.0593
 32.0611    58.7851    81.0125   …  -38.534    -25.8457   ␣
↪-12.9839
 31.8182    58.1704    79.8576      -41.5677   -27.8638   ␣
↪-13.99
 30.4662    55.6291    76.1784      -44.7712   -30.0171   ␣
↪-15.0775

-15.732    -30.7192   -44.9899      -57.312    -38.9096   ␣
↪-19.819
-14.7362   -28.7298   -42.011    …  -53.6836   -36.4846   ␣
↪-18.6046
-13.714    -26.6883   -38.9555      -49.9246   -33.9713   ␣
↪-17.3457
-12.6627   -24.5893   -35.8159      -46.0225   -31.3611   ␣
↪-16.0379
-11.5784   -22.4259   -32.5829      -41.9624   -28.6434   ␣
↪-14.6757
-10.4561   -20.1885   -29.2437      -37.7261   -25.8053   ␣
↪-13.2523
 -9.28854  -17.8638   -25.7807   …  -33.2908   -22.8302   ␣
↪-11.7589
```

```
 -8.06529  -15.4329   -22.1697      -28.6277   -19.6966  ␣
↪-10.184
 -6.77073  -12.8683   -18.3765      -23.699    -16.3753  ␣
↪-8.51129
 -5.38033  -10.1287   -14.3517      -18.4544   -12.8253  ␣
↪-6.71668
 -3.85295   -7.14974  -10.0239      -12.8253    -8.98543 ␣
↪-4.76102
 -2.11273   -3.829     -5.28902  …   -6.71668   -4.76102 ␣
↪-2.5728
```

[27]:
```
p_pot = surface(rhs_xs, rhs_ys, sol, xlabel=L"X",␣
↪ylabel=L"Y", colorbar=:none)
```

[27]:



Helper function to compute 2D histograms for Probability distributions

[28]:
```
begin
        nbins = 701
        bin_min = 0
        bin_max = 700
```

```
        xbins = range(bin_min, bin_max, length=nbins)
        ybins = range(bin_min, bin_max, length=nbins)

        function bucket_idx(val, vec)
                idx = 1
                while val > vec[idx]
                        idx += 1
                end
                idx
        end

        function althist(x, y, dt, xedges, yedges)
           counts = spzeros(length(yedges)-1,␣
↪length(xedges)-1)
                for i=1:length(x) - 1
                        r = bucket_idx(y[i], yedges)
                        c = bucket_idx(x[i], xedges)
                        counts[r,c] += dt[i]
                end
                 counts
        end
end
```

[28]:
```
althist (generic function with 1 method)
```

Storage for unnormalized probabilities that sum up the `dt`*s in each bin*

[29]:
```
begin
        unnorm_ssa = spzeros(length(xbins)-1,␣
↪length(ybins)-1)
        unnorm_sde = spzeros(length(xbins)-1,␣
↪length(ybins)-1)
        tspan = (0., 5e4)
end
```

[29]:
```
(0.0, 50000.0)
```

Rerun the following cell to add more values to the SSA simulation

[30]:
```
begin
        global n_points_sim
        for i in 1:3*10
                long_jprob_ssa = JumpProblem(
                        DiscreteProblem(get_u0(i), tspan),␣
↪Direct(), constJumps...)
                long_ssa_sol = solve(long_jprob_ssa,␣
↪SSAStepper())
                unnorm_ssa .+= althist(long_ssa_sol[1,:],␣
↪long_ssa_sol[2, :], diff(long_ssa_sol.t[:]), xbins, ybins)
        end
        unnorm_ssa
end
```

[30]:
```
700×700 SparseMatrixCSC{Float64, Int64} with 31740 stored␣
↪entries:
```

Rerun the following cell to have the SDE simulation catch up to the SSA

[31]:
```
begin
        i = 1
        num_sde_run_failures = 0
        while sum(unnorm_sde) < sum(unnorm_ssa)
                global i
                global num_sde_run_failures


                sde_run = SDEProblem(f, g, get_u0(i), tspan,␣
 ↪noise_rate_prototype=zeros(2,4))
                sol = solve(sde_prob_ssa)

                if sol.t[end] < tspan[end]
                        # the simulation did not complete␣
 ↪succesfully.
                        # This is a sign of divergence and a␣
 ↪failing approximation
                        num_sde_run_failures += 1
                end
                unnorm_sde .+= althist(sol[1,:], sol[2, :],␣
 ↪diff(sol.t[:]), xbins, ybins)
                i += 1
        end
        unnorm_sde, num_sde_run_failures, i
end
```

```
 Warning: dt <= dtmin. Aborting. There is either an error in␣
 ↪your model
specification or the true solution is unstable.
 @ SciMLBase
/Users/bsm/.julia/packages/SciMLBase/EFFG1/src/
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```

```
[31]: (
```

```
, 93, 94)
```

[32]:
```
prob_ssa = unnorm_ssa ./ sum(unnorm_ssa)
```

[32]:
```
700×700 SparseMatrixCSC{Float64, Int64} with 31740 stored␣
↪entries:
```

[39]:
```
prob_sde = unnorm_sde ./ sum(unnorm_sde)
```

[39]:
```
700×700 SparseMatrixCSC{Float64, Int64} with 33705 stored␣
↪entries:
```

the SDE probability distribution is complete non-sense

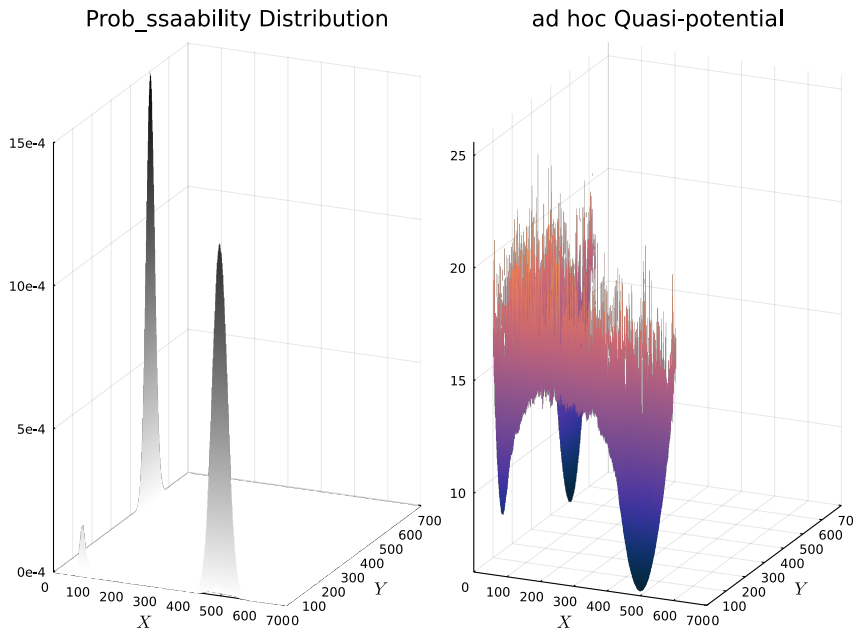
[40]:
```
begin
        plotly()
        pl = surface(prob_sde, xlabel="X", ylabel="Y")
        gr()
        pl
end
```

[35]:
```
begin
        xplot = range(bin_min, bin_max, length=nbins-1)
        yplot = range(bin_min, bin_max, length=nbins-1)
end
```

[35]:
```
0.0:1.0014306151645207:700.0
```

[37]:
```
begin
        pp1 = surface(xplot, yplot,-log.(prob_ssa), c = :
 ↪thermal, title="ad hoc Quasi-potential")
        pp2 =  surface(xplot, yplot, prob_ssa, c = :grayC,␣
 ↪title="Prob_ssaability Distribution",␣
 ↪zaxis=(formatter=y->string(round(Int, y / 10^-4))*"e-4" )␣
 ↪)
        ps = plot(pp2, pp1, layout =(1, 2), size=(800, 600),␣
 ↪xlabel=L"X", ylabel=L"Y", colorbar=:none)
end
```

[37]:



[ ]: