

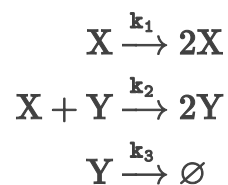
```

1 begin
2   # numerical libraries
3   using Expokit, PROPACK, Arpack, SparseArrays
4   # output and plotting
5   using ProgressLogging, JLD, CairoMakie
6   # modelling and statistics
7   using Catalyst, JumpProcesses, StatsBase, DifferentialEquations
8   using Interpolations
9   # importing local fsp package
10  using Revise
11  local_mod = include("../src/DiscStochSim.jl")
12  using .local_mod.DiscStochSim
13 end

```

Replacing docs for `Main.var"workspace#2".DiscStochSim.FindLowestValuesPercent` :
 : Union{Tuple{T}, Tuple{Vector{T}, Number}} where T` in module `Main.var"workspace#2".DiscStochSim`

rn =



```

1 rn = @reaction_network begin
2   k1, X --> 2X
3   k2, X + Y --> 2Y
4   k3, Y --> 0
5 end

```

```
1 model = DiscreteStochasticSystem(rn);
```

def_params = 0.0:0.005:30.0

```

1 def_params = begin
2   # reaction rates
3   rates = [1.0, 0.005, 0.6]
4   # boundary
5   bounds = (0, 500)  #(lower limit, upper limit)
6   boundary_condition(x) = RectLatticeBoundaryCondition(x, bounds);
7   # time interval and initial values
8   dt = 0.005
9   T = 0:dt:30
10 end

```

Initialize Finite State Space

```

1 init_fsp_vars = begin
2   global U0 = CartesianIndex(50, 100)
3   global S0 = Set([U0])
4   global S0 = expand!(S0, model, rates, 0.0, boundary_condition, 1);
5   # initial probability vector (only for active states)
6   global p0 = zeros(S0 |> length)
7   global p0[FindElement(U0, S0)] = 1
8 end;

```

fsp_sim =

```

1 fsp_sim = begin
2   # copy initial values
3   pt = copy(p0)
4   St = copy(S0)
5   # time stepping loop
6   iter = 1
7   pt = p0
8   # variables to store simulation observables
9   size_St = Int.(zeros(length(I))) # system sizes
10  et = zeros(length(I)) # local truncation err
11  sol = Array{SparseMatrixCSC,1}(undef, length(I))
12  @progress for (iter, t) ∈ enumerate(I)
13    # expand state space
14    global St, pt = expand!(St, pt, model, rates, t, boundary_condition, 3)
15    global size_St[iter] = length(St)
16    A = MasterEquation(St, model, rates, boundary_condition, t)
17    # solve system and normalize (using expokit)
18    global pt = expmv(δt, A, pt)
19    # add add states in sparse arrays
20    I = [a[1] for a in St]
21    J = [a[2] for a in St]
22    global sol[iter] = sparse(I, J, pt)
23    # purge state space
24    St, pt = purge!(St, pt, 3.0)
25    et[iter] = 1.0 - sum(pt)
26    pt ./= sum(pt)
27  end
28 end

```

100%

FSP Mean Trajectory

Since the solution computed by the FSP algorithm is

$$X_{mean} = \sum_{i=0}^N X_i \cdot p(X_i, t)$$

```
1 compute_fsp_mean = begin
2   cart2vec(x) = [Tuple(x)...]
3   sol_mean = map(1:length(I)) do i
4     I, J, V = findnz(sol[i])
5     sum(hcat(I, J) .* V, dims=1)
6   end
7
8   x = @inbounds [sol_mean[i][1] for i ∈ 1:length(sol_mean)]
9   y = @inbounds [sol_mean[i][2] for i ∈ 1:length(sol_mean)]
10  fsp_mean = hcat(x, y);
11 end;
```

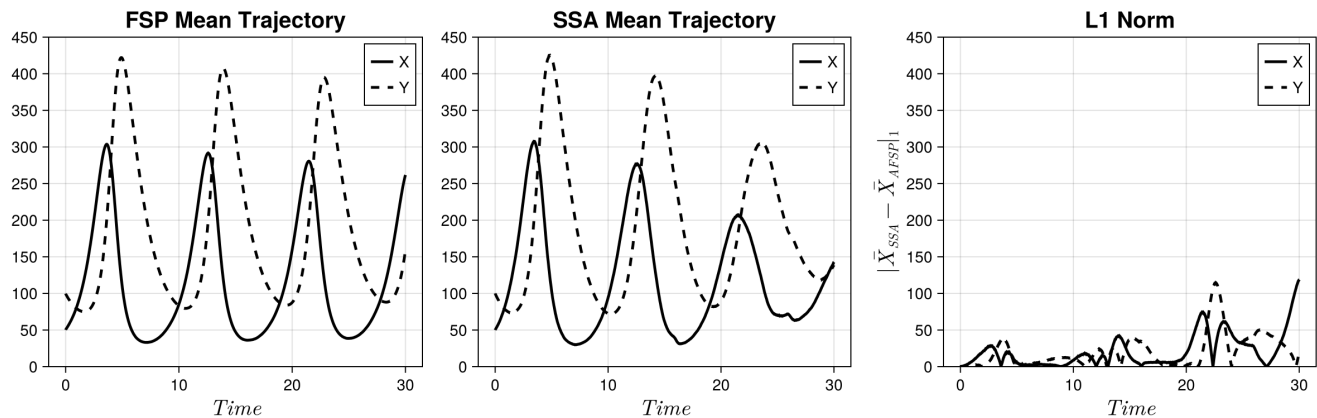
Generate SSA Trajectories

We use jump processes

```
generate_ssa_samples =
1 generate_ssa_samples = begin
2     # Create an ODE that can be simulated.
3     u0_integers = [:X => 50, :Y => 100]
4     ps = [:k1 => 1.0, :k2 => 0.005, :k3 => 0.6]
5     tspan = (0., 30.)
6
7     jinput = JumpInputs(rn, u0_integers, tspan, ps)
8     jprob = JumpProblem(jinput)
9     jump_sol = solve(jprob)
10
11     n_trajs = 300 # increase for a more accurate ssa mean
12     ssa_trajs1=[]
13     @progress for i in 1:n_trajs
14         push!(ssa_trajs1, solve(jprob, SSAS stepper()))
15     end;
16 end
```

100%

```
1 uniform_time, ssa_mean = mean_trajectory(ssa_trajs1, I[1], I[end], length(I));
```



```
1 @save "lv_data.jld" sol, εt size_St
```