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

Replacing docs for `Main.var"workspace#4".DiscStochSim.FindLowestValuesPercent :
: Union{Tuple{T}, Tuple{Vector{T}, Number}} where T` in module `Main.var"workspa
ce#4".DiscStochSim`

rn =

$$S + E \underset{kD}{\overset{kB}{\rightleftharpoons}} SE$$

$$SE \xrightarrow{kP} P + E$$

```
1 rn = @reaction_network begin
2     kB, S + E --> SE
3     kD, SE --> S + E
4     kP, SE --> P + E
5 end
```

```
1 model = DiscreteStochasticSystem(<u>rn</u>);
```

```
def_params = 0.0:0.01:200.0
```

```
def_params = begin
    # reaction rates
    rates = [0.01, 0.1, 0.1];

# boundary
bounds = (0, 60) #(lower limit, upper limit)
boundary_condition(x) = RectLatticeBoundaryCondition(x, bounds);

# time interval and initial values

8 δt = 0.01
T = 0:δt:200

10 end
```

```
init_fsp_vars = begin
global U<sub>0</sub> = CartesianIndex(50, 10, 1, 1);
global S<sub>0</sub> = Set([U<sub>0</sub>])
global S<sub>0</sub> = expand!(S<sub>0</sub>, model, rates, 0.0, boundary_condition, 1);
# initial probability vector (only for active states)
global p<sub>0</sub> = zeros(S<sub>0</sub> |> length)
global p<sub>0</sub>[FindElement(U<sub>0</sub>, S<sub>0</sub>)] = 1
end;
```

```
fsp_sim =
 1 fsp_sim = begin
 2
 3
         # copy initial values
 4
         p_t = copy(\underline{p_0})
 5
         S_t = \text{copy}(\underline{S_0})
 6
 7
         # time stepping loop
 8
         iter = 1
 9
         p_t = p_0
10
11
         # variables to store simulation observables
12
         size_S_t = Int.(zeros(length(\underline{T}))) # system sizes
13
         \epsilon_t = zeros(length(\underline{T})) #local truncation err
14
         sol = []
15
16
         Qprogress for (iter, t) \in enumerate(\underline{T})
17
18
              # expand state space
              global S_t, p_t = expand! (S_t, p_t, model, rates, t, boundary_condition, 3)
19
20
              global size_S_t[iter] = length(S_t)
              A = MasterEquation(S_t, model, rates, boundary_condition, t)
21
22
23
              # solve system and normalize (using expokit)
24
              global p_t = expmv(\underline{\delta t}, A, p_t)
25
26
              # add add states in sparse arrays
27
              push!(sol, (S_t, p_t))
28
29
              # purge state space
30
             S_{t}, p_{t} = purge!(S_{t}, p_{t}, 3.0)
31
              \epsilon_t[iter] = 1.0 - sum(p_t)
32
              p_t ./= sum(p_t)
33
         end
34
35 end
```

100%

```
20001×4 adjoint(::Matrix{Float64}) with eltype Float64:
          9.95607 1.04393 1.00002
49.914
          9.91402 1.08598
                            1.0
49.8752
         9.87521
                   1.12479
                            1.0
49.8393
         9.83929
                  1.16071
                            1.0
49.8059
         9.80594
                  1.19406
                           1.0
49.7749
         9.77491
                  1.22509
                           1.0
49.746
         9.74596 1.25404
                           1.0
47.1873
         7.1873
                   3.8127
                            1.00004
47.1876
         7.18768
                  3.81232
                            1.00004
        7.18964
47.1869
                   3.81036 1.00275
47.187
         7.18699
                  3.81301 1.0
47.187
          7.18695
                  3.81305
                            1.0
47.1873 7.18734 3.81266
                            1.0
 1 begin
       sol_mean = map(1:length(\underline{T})) do i
 2
           sum(collect.(Tuple.(sol[i][1])) .* sol[i][2])
 4
       end
 5
       fsp_mean=hcat(sol_mean...)'
 6 end
```

```
1 begin
 2
        u0_integers = [:S => 50, :E => 10, :SE => 1, :P => 1]
 3
        tspan = (0., 200.)
 4
        ps = [:kB \Rightarrow 0.01, :kD \Rightarrow 0.1, :kP \Rightarrow 0.1]
 5
 6
        jinput = JumpInputs(<u>rn</u>, u0_integers, tspan, ps)
 7
        jprob = JumpProblem(jinput)
 8
        jump_sol = solve(jprob; seed=1234)
 9
10
        n_{trajs} = 1000
11
        ssa_trajs1=[]
        @progress for i in 1:n_trajs
12
13
            push!(ssa_trajs1, solve(jprob, SSAStepper()))
14
15 end
```

100%

```
(20001-element LinRange{Float64, Int64}:
0.0. 0.01. 0.02. 0.03. 0.04. 0.05. 0.06. ... 199.96. 199.97. 199.98. 199.99. 200.0 50

1 uniform_time, ssa_mean = mean_trajectory(<u>ssa_trajs1</u>, 0.0, 200.0, length(<u>T</u>))
```

