Finding Maxima and Minima of DiffEq Solutions

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0.0.1 Setup

In this tutorial we will show how to use Optim.jl to find the maxima and minima of solutions. Let's take a look at the double pendulum:

```
#Constants and setup
using OrdinaryDiffEq
initial = [0.01, 0.01, 0.01, 0.01]
tspan = (0.,100.)

#Define the problem
function double_pendulum_hamiltonian(udot,u,p,t)
    α  = u[1]
    lα = u[2]
    β  = u[3]
    lβ = u[4]
    udot .=
    [2(lα-(1+cos(β))lβ)/(3-cos(2β)),
    -2sin(α) - sin(α+β),
    2(-(1+cos(β))lα + (3+2cos(β))lβ)/(3-cos(2β)),
    -sin(α+β) - 2sin(β)*(((lα-lβ)lβ)/(3-cos(2β))) + 2sin(2β)*((lα^2 - 2(1+cos(β))lα*lβ
    + (3+2cos(β))lβ^2)/(3-cos(2β))^2)]
end

#Pass to solvers
poincare = ODEProblem(double_pendulum_hamiltonian, initial, tspan)
```

```
ODEProblem with uType Array{Float64,1} and tType Float64. In-place: true
timespan: (0.0, 100.0)
u0: [0.01, 0.01, 0.01, 0.01]
```

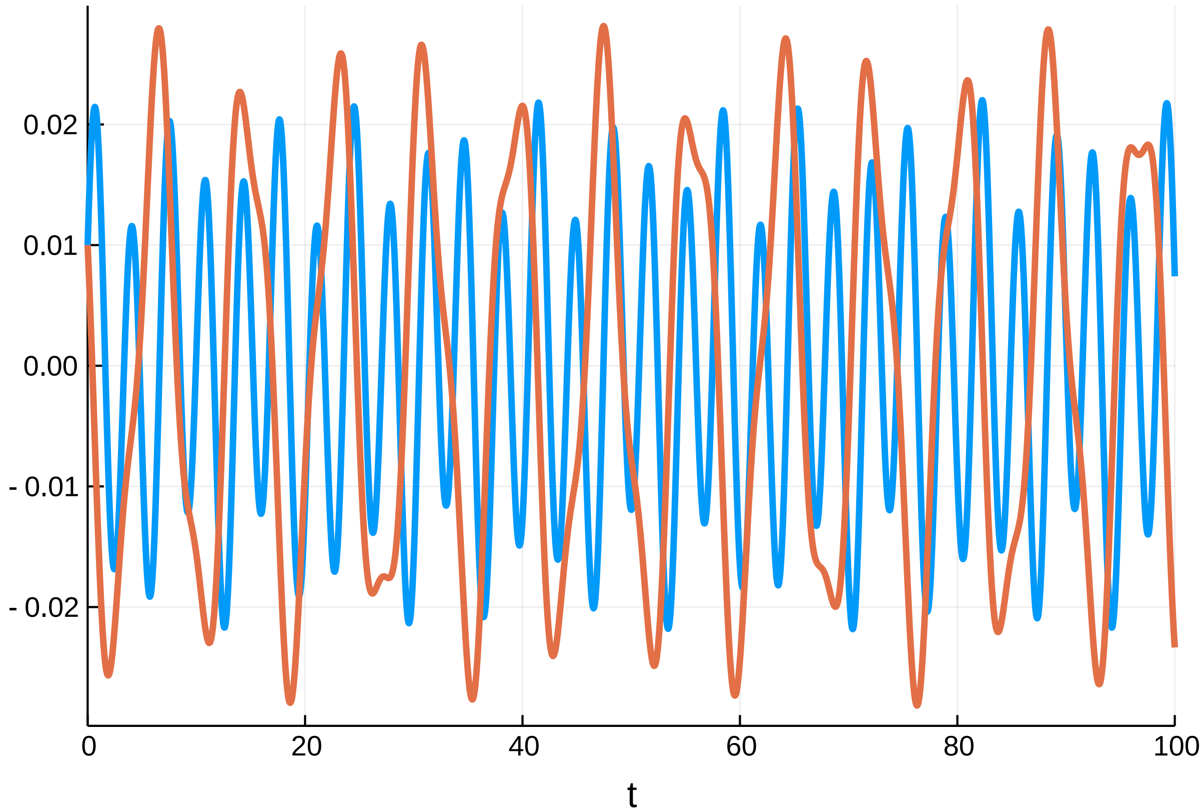
```
sol = solve(poincare, Tsit5())
```

```
retcode: Success
Interpolation: specialized 4th order "free" interpolation
t: 193-element Array{Float64,1}:
   0.0
   0.08332584852065579
```

```
   0.24175280272193683
   0.438953650048967
   0.679732254249109
   0.9647633763375199
   1.317944955684634
   1.7031210236334697
   2.067847793204029
   2.4717825254408226
   ⋮
  95.84571836675161
  96.35777612654947
  96.9291238553289
  97.44678729813481
  97.96247442963697
  98.5118249699588
  99.06081878698636
  99.58283477685136
 100.0
u: 193-element Array{Array{Float64,1},1}:
 [0.01, 0.01, 0.01, 0.01]
 [0.00917069, 0.006669, 0.0124205, 0.00826641]
 [0.00767328, 0.000374625, 0.0164426, 0.00463683]
 [0.00612597, -0.00730546, 0.0199674, -0.000336506]
 [0.0049661, -0.0163086, 0.0214407, -0.00670509]
 [0.00479557, -0.0262381, 0.0188243, -0.0139134]
 [0.00605469, -0.0371246, 0.0100556, -0.0210382]
 [0.00790078, -0.046676, -0.00267353, -0.025183]
 [0.00827652, -0.0527843, -0.0127315, -0.0252581]
 [0.00552358, -0.0552525, -0.0168439, -0.021899]
 ⋮
 [-0.0148868, 0.0423324, 0.0136282, 0.0180291]
 [-0.00819054, 0.0544225, 0.00944831, 0.0177401]
 [0.00412448, 0.0567489, -0.00515392, 0.017597]
 [0.0130796, 0.0480772, -0.0137706, 0.0182866]
 [0.0153161, 0.0316313, -0.00895722, 0.0171185]
 [0.0111156, 0.00992938, 0.0072972, 0.0103535]
 [0.00571392, -0.0117872, 0.020508, -0.00231029]
 [0.00421143, -0.0299109, 0.0187506, -0.0156505]
 [0.00574124, -0.0416539, 0.00741327, -0.023349]
```

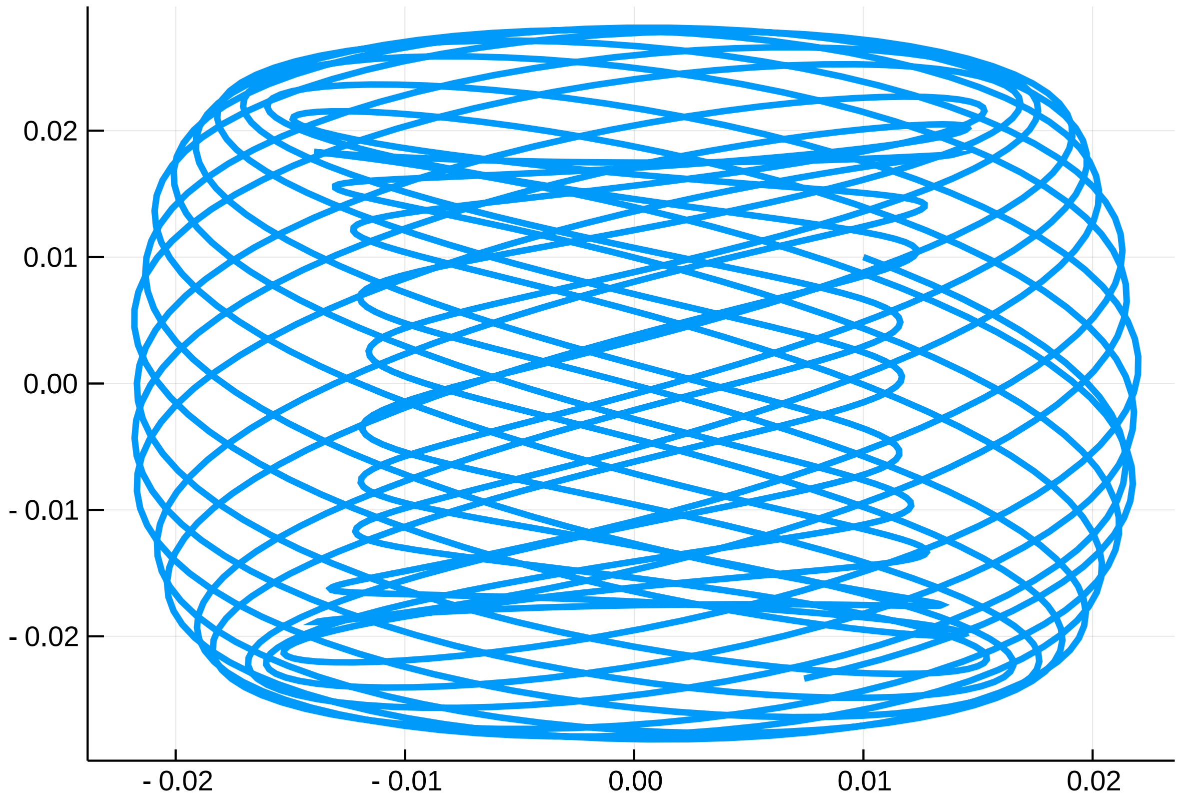
In time, the solution looks like:

```
using Plots; gr()
plot(sol, vars=[(0,3),(0,4)], leg=false, plotdensity=10000)
```



while it has the well-known phase-space plot:

```
plot(sol, vars=(3,4), leg=false)
```



0.0.2 Local Optimization

Let's fine out what some of the local maxima and minima are. Optim.jl can be used to minimize functions, and the solution type has a continuous interpolation which can be used. Let's look for the local optima for the 4th variable around `t=20`. Thus our optimization function is:

```
f = (t) -> sol(t,idxs=4)
```

```
#1 (generic function with 1 method)
```

`first(t)` is the same as `t[1]` which transforms the array of size 1 into a number. `idxs=4` is the same as `sol(first(t))[4]` but does the calculation without a temporary array and thus is faster. To find a local minima, we can simply call Optim on this function. Let's find a local minimum:

```
using Optim
opt = optimize(f,18.0,22.0)
```

```
Results of Optimization Algorithm
 * Algorithm: Brent's Method
 * Search Interval: [18.000000, 22.000000]
 * Minimizer: 1.863213e+01
 * Minimum: -2.793164e-02
 * Iterations: 11
 * Convergence: max(|x - x_upper|, |x - x_lower|) <= 2*(1.5e-08*|x|+2.2e-16
): true
 * Objective Function Calls: 12
```

From this printout we see that the minimum is at `t=18.63` and the value is `-2.79e-2`. We can get these in code-form via:

```
println(opt.minimizer)
```

```
18.632126799604933
```

```
println(opt.minimum)
```

```
-0.027931635264245896
```

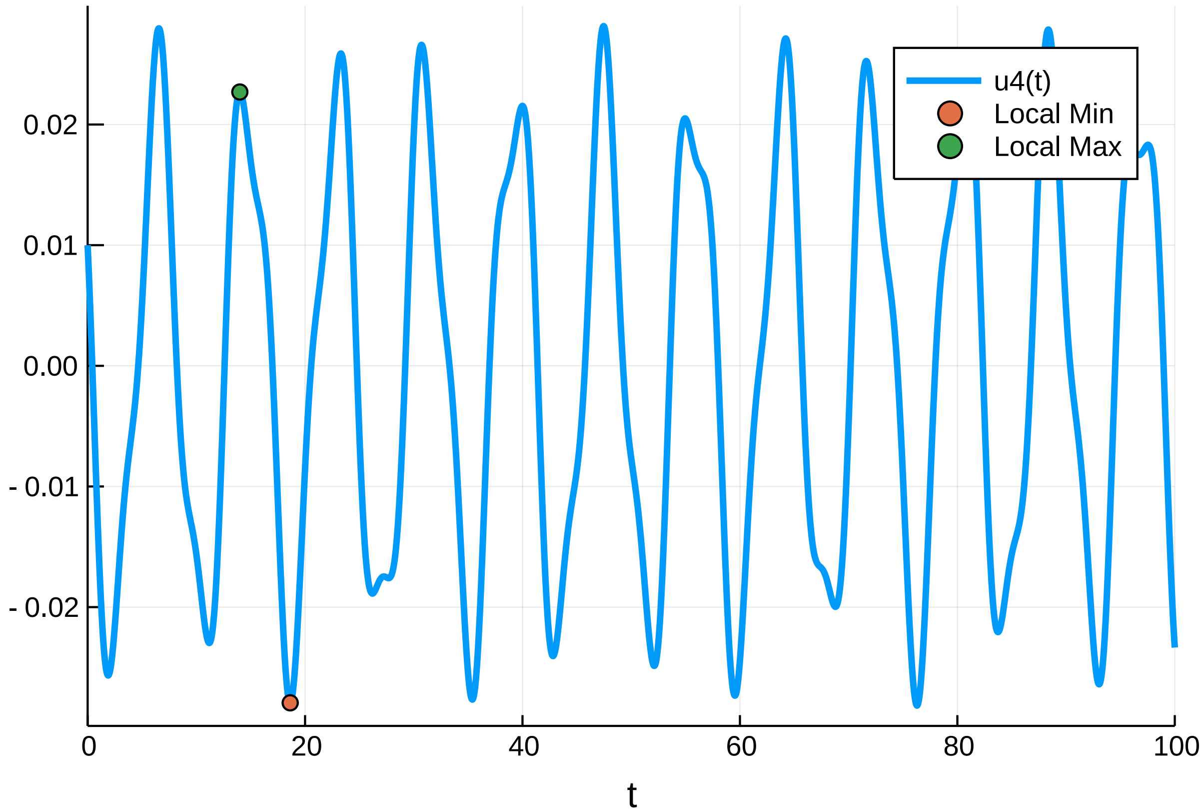
To get the maximum, we just minimize the negative of the function:

```
f = (t) -> -sol(first(t),idxs=4)
opt2 = optimize(f,0.0,22.0)
```

```
Results of Optimization Algorithm
 * Algorithm: Brent's Method
 * Search Interval: [0.000000, 22.000000]
 * Minimizer: 1.399975e+01
 * Minimum: -2.269411e-02
 * Iterations: 13
 * Convergence: max(|x - x_upper|, |x - x_lower|) <= 2*(1.5e-08*|x|+2.2e-16
): true
 * Objective Function Calls: 14
```

Let's add the maxima and minima to the plots:

```
plot(sol, vars=(0,4), plotdensity=10000)
scatter!([opt.minimizer],[opt.minimum],label="Local Min")
scatter!([opt2.minimizer],[-opt2.minimum],label="Local Max")
```



Brent's method will locally minimize over the full interval. If we instead want a local maxima nearest to a point, we can use `BFGS()`. In this case, we need to optimize a vector `[t]`, and thus dereference it to a number using `first(t)`.

```
f = (t) -> -sol(first(t),idxs=4)
opt = optimize(f,[20.0],BFGS())
```

```
Results of Optimization Algorithm
 * Algorithm: BFGS
 * Starting Point: [20.0]
```

```
 * Minimizer: [23.29760728871635]
 * Minimum: -2.588588e-02
 * Iterations: 4
 * Convergence: true
   * |x - x'| ≤ 0.0e+00: false
     |x - x'| = 1.11e-04
   * |f(x) - f(x')| ≤ 0.0e+00 |f(x)|: false
     |f(x) - f(x')| = -6.49e-09 |f(x)|
   * |g(x)| ≤ 1.0e-08: true
     |g(x)| = 8.42e-12
   * Stopped by an increasing objective: false
   * Reached Maximum Number of Iterations: false
 * Objective Calls: 16
 * Gradient Calls: 16
```

0.0.3 Global Optimization

If we instead want to find global maxima and minima, we need to look somewhere else. For this there are many choices. A pure Julia option is BlackBoxOptim.jl, but I will use NLopt.jl. Following the NLopt.jl tutorial but replacing their function with out own:

```
import NLopt, ForwardDiff

count = 0 # keep track of # function evaluations

function g(t::Vector, grad::Vector)
  if length(grad) > 0
    #use ForwardDiff for the gradients
    grad[1] = ForwardDiff.derivative((t)->sol(first(t),idxs=4),t)
  end
  sol(first(t),idxs=4)
end
opt = NLopt.Opt(:GN_ORIG_DIRECT_L, 1)
NLopt.lower_bounds!(opt, [0.0])
NLopt.upper_bounds!(opt, [40.0])
NLopt.xtol_rel!(opt,1e-8)
NLopt.min_objective!(opt, g)
(minf,minx,ret) = NLopt.optimize(opt,[20.0])
println(minf," ",minx," ",ret)
```

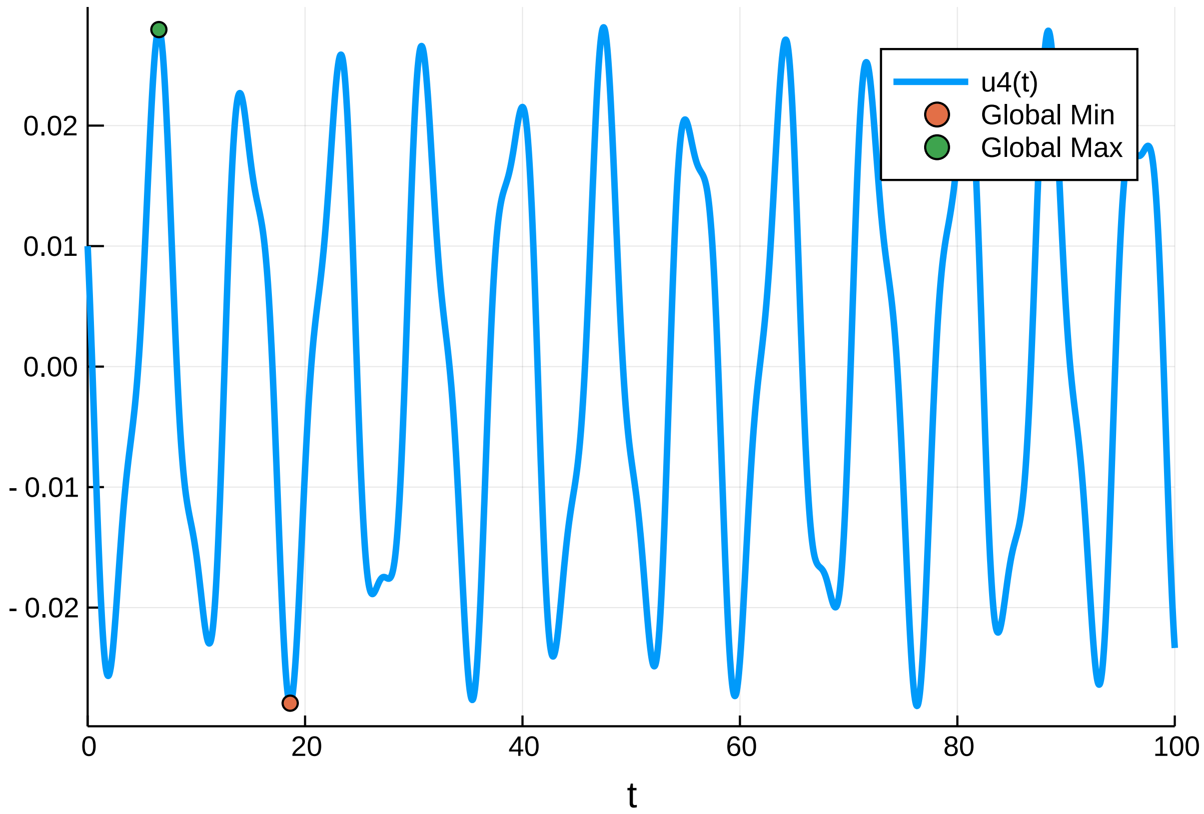
```
-0.027931635264245837 [18.6321] XTOL_REACHED
```

```
NLopt.max_objective!(opt, g)
(maxf,maxx,ret) = NLopt.optimize(opt,[20.0])
println(maxf," ",maxx," ",ret)
```

```
0.027968571933041954 [6.5537] XTOL_REACHED
```

```
plot(sol, vars=(0,4), plotdensity=10000)
```

```
scatter!([minx],[minf],label="Global Min")
scatter!([maxx],[maxf],label="Global Max")
```




```
using DiffEqTutorials
DiffEqTutorials.tutorial_footer(WEAVE_ARGS[:folder],WEAVE_ARGS[:file])
```

0.1 Appendix

These benchmarks are part of the DiffEqTutorials.jl repository, found at: https://github.com/JuliaDiffEq/

To locally run this tutorial, do the following commands:

```
using DiffEqTutorials
DiffEqTutorials.weave_file("ode_extras","ode_minmax.jmd")
```

Computer Information:

```
Julia Version 1.1.0
Commit 80516ca202 (2019-01-21 21:24 UTC)
Platform Info:
  OS: Windows (x86_64-w64-mingw32)
  CPU: Intel(R) Core(TM) i7-8700 CPU @ 3.20GHz
  WORD_SIZE: 64
  LIBM: libopenlibm
  LLVM: libLLVM-6.0.1 (ORCJIT, skylake)
```

```
Environment:
  JULIA_EDITOR = "C:\Users\accou\AppData\Local\atom\app-1.34.0\atom.exe" -a
  JULIA_NUM_THREADS = 6
```

Package Information:

```
Status `C:\Users\accou\.julia\environments\v1.1\Project.toml`
[7e558dbc-694d-5a72-987c-6f4ebed21442] ArbNumerics 0.3.6
[c52e3926-4ff0-5f6e-af25-54175e0327b1] Atom 0.7.14
[6e4b80f9-dd63-53aa-95a3-0cdb28fa8baf] BenchmarkTools 0.4.2
[336ed68f-0bac-5ca0-87d4-7b16caf5d00b] CSV 0.4.3
[3895d2a7-ec45-59b8-82bb-cfc6a382f9b3] CUDAapi 0.6.0
[be33ccc6-a3ff-5ff2-a52e-74243cff1e17] CUDAnative 1.0.1
[3a865a2d-5b23-5a0f-bc46-62713ec82fae] CuArrays 0.9.1
[a93c6f00-e57d-5684-b7b6-d8193f3e46c0] DataFrames 0.17.1
[55939f99-70c6-5e9b-8bb0-5071ed7d61fd] DecFP 0.4.8
[abce61dc-4473-55a0-ba07-351d65e31d42] Decimals 0.4.0
[bcd4f6db-9728-5f36-b5f7-82caef46ccdb] DelayDiffEq 5.2.0+
[39dd38d3-220a-591b-8e3c-4c3a8c710a94] Dierckx 0.4.1
[2b5f629d-d688-5b77-993f-72d75c75574e] DiffEqBase 5.4.0+
[bb2cbb15-79fc-5d1e-9bf1-8ae49c7c1650] DiffEqBenchmarks 0.0.0
[459566f4-90b8-5000-8ac3-15dfb0a30def] DiffEqCallbacks 2.5.2
[f3b72e0c-5b89-59e1-b016-84e28bfd966d] DiffEqDevTools 2.6.1
[aae7a2af-3d4f-5e19-a356-7da93b79d9d0] DiffEqFlux 0.2.0
[c894b116-72e5-5b58-be3c-e6d8d4ac2b12] DiffEqJump 6.1.0+
[1130ab10-4a5a-5621-a13d-e4788d82bd4c] DiffEqParamEstim 1.6.0+
[055956cb-9e8b-5191-98cc-73ae4a59e68a] DiffEqPhysics 3.1.0
[a077e3f3-b75c-5d7f-a0c6-6bc4c8ec64a9] DiffEqProblemLibrary 4.1.0
[225cb15b-72e6-54e6-9a40-306d353791de] DiffEqTutorials 0.0.0
[0c46a032-eb83-5123-abaf-570d42b7fbaa] DifferentialEquations 6.3.0
[497a8b3b-efae-58df-a0af-a86822472b78] DoubleFloats 0.7.5
[587475ba-b771-5e3f-ad9e-33799f191a9c] Flux 0.7.3
[f6369f11-7733-5829-9624-2563aa707210] ForwardDiff 0.10.3+
[28b8d3ca-fb5f-59d9-8090-bfdbd6d07a71] GR 0.38.1
[7073ff75-c697-5162-941a-fcdaad2a7d2a] IJulia 1.17.0
[c601a237-2ae4-5e1e-952c-7a85b0c7eef1] Interact 0.9.1
[b6b21f68-93f8-5de0-b562-5493be1d77c9] Ipopt 0.5.4
[4076af6c-e467-56ae-b986-b466b2749572] JuMP 0.19.0
[e5e0dc1b-0480-54bc-9374-aad01c23163d] Juno 0.5.4
[7f56f5a3-f504-529b-bc02-0b1fe5e64312] LSODA 0.4.0
[eff96d63-e80a-5855-80a2-b1b0885c5ab7] Measurements 2.0.0
[76087f3c-5699-56af-9a33-bf431cd00edd] NLopt 0.5.1
[c030b06c-0b6d-57c2-b091-7029874bd033] ODE 2.4.0
[54ca160b-1b9f-5127-a996-1867f4bc2a2c] ODEInterface 0.4.5+
[09606e27-ecf5-54fc-bb29-004bd9f985bf] ODEInterfaceDiffEq 3.0.0
[429524aa-4258-5aef-a3af-852621145aeb] Optim 0.17.2
[1dea7af3-3e70-54e6-95c3-0bf5283fa5ed] OrdinaryDiffEq 5.3.0+
[65888b18-ceab-5e60-b2b9-181511a3b968] ParameterizedFunctions 4.1.1
```

```
[91a5bcdd-55d7-5caf-9e0b-520d859cae80] Plots 0.23.0
[71ad9d73-34c4-5ce9-b7b1-f7bd31ac38ba] PuMaS 0.0.0
[d330b81b-6aea-500a-939a-2ce795aea3ee] PyPlot 2.7.0
[731186ca-8d62-57ce-b412-fbd966d074cd] RecursiveArrayTools 0.20.0
[90137ffa-7385-5640-81b9-e52037218182] StaticArrays 0.10.2
[789caeaf-c7a9-5a7d-9973-96adeb23e2a0] StochasticDiffEq 6.1.1+
[c3572dad-4567-51f8-b174-8c6c989267f4] Sundials 3.1.0+
[1986cc42-f94f-5a68-af5c-568840ba703d] Unitful 0.14.0
[2a06ce6d-1589-592b-9c33-f37faeaed826] UnitfulPlots 0.0.0
[44d3d7a6-8a23-5bf8-98c5-b353f8df5ec9] Weave 0.7.2
```