Implementation of implicit integrators in Matlab/Octave

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Passing parameters to functions

 Matlab functions take formal arguments, but sometimes we need to pass a parameter to a function in a way that is invisible, perhaps because the function is to be used as a function argument itself.

Method 1: Declare the parameter to be global.

global k m

Put this line both in the main script before assigning values to the parameters, and in the function.

Method 2: Anonymous functions

0(x)f(x,k)

This creates a new function of x from a function that actually depends on both x and k.

Iterative solution method

• Equations to solve for (x_{j+1}, p_{j+1}) :

$$\frac{x_{j+1} - x_j}{h} = \frac{H(x_j, p_{j+1}) - H(x_j, p_j)}{p_{j+1} - p_j}$$
$$\frac{p_{j+1} - p_j}{h} = -\frac{H(x_{j+1}, p_{j+1}) - H(x_j, p_{j+1})}{x_{j+1} - x_j}$$

Rewrite in the Euler-like form

$$x_{j+1} = x_j + h \frac{H(x_j, p_{j+1}) - H(x_j, p_j)}{p_{j+1} - p_j}$$
$$p_{j+1} = p_j - h \frac{H(x_{j+1}, p_{j+1}) - H(x_j, p_{j+1})}{x_{j+1} - x_j}$$

Iterative solution method

$$x_{j+1} = x_j + h \frac{H(x_j, p_{j+1}) - H(x_j, p_j)}{p_{j+1} - p_j}$$
 (1a)

$$p_{j+1} = p_j - h \frac{H(x_{j+1}, p_{j+1}) - H(x_j, p_{j+1})}{x_{j+1} - x_j}$$
 (1b)

- Problem: x_{i+1} and p_{i+1} both appear in the right-hand sides of these equations.
- Generate a guess for x_{i+1} and p_{i+1} using an explicit method, then substitute this guess into equations (1) to refine this approximate solution.
 - Iterate until the variables change negligibly from one iteration to the next.

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Using fsolve()

- Instead of solving the equations yourself by iteration, you can use the Matlab/Octave function fsolve().
- Warning: In Matlab, fsolve() is part of the Optimization Toolbox. It may not be available in a "vanilla" Matlab installation.
- Syntax:

Assumption: you want to solve the equation f(v) = 0, where v is a vector containing your variables.

v0 is an initial guess vector.

On output, v is the solution.

fsolve options

 The options used by fsolve have different names in Matlab and Octave.

FunctionTolerance (Matlab)/TolFun (Octave) is the maximum value of f required for the algorithm to stop.

StepTolerance (Matlab)/TolX (Octave) is the maximum difference between one iterate and the next for the algorithm to stop.

- An option structure is created by optimset().
 opts = optimset('TolX',1e-8,'TolFun',1e-4);
- An option structure (e.g. opts above) is passed as the final argument of fsolve().