Complex-Step Derivative Approximations for Sensitivity Analysis

Ralph C. Smith
Department of Mathematics
North Carolina State University

Local Sensitivity Sensitivity Analysis

Motivation:

- Ascertain whether the model is robust or overly fragile with regard to various parameters;
- Determine whether the model can be simplified by fixing insensitive parameters;
- Specify regimes in the parameter space that optimally impact responses or their uncertainties;
- Guide experimental design to determine measurement regimes that have the greatest impact on parameter or response sensitivity.

Models:

$$y = f(\theta)$$

$$y = f(t, \theta)$$

$$y_i = f(t_i, \theta)$$

$$y_i = f(t_i, \theta) + \varepsilon_i$$

Notation:

y : Vector or scalar-valued response

θ : Inputs; e.g., parameters, IC, BC

t : Independent variable; e.g., time

ε_i : Observation errors

Complex-Step Derivative Approximation

Initial Approach: Consider complex variable $z = x + iy$ and function $f(z) = u(x, y) + iv(x, y)$. For *analytic* f, consider Cauchy-Riemann equations

$$\frac{\partial u}{\partial x} = \frac{\partial v}{\partial y} \quad , \quad \frac{\partial u}{\partial y} = -\frac{\partial v}{\partial x}$$

For real h,

$$\begin{aligned} \frac{\partial u}{\partial x} &= \lim_{h \to 0} \frac{v(x, y + h) - v(x, y)}{h} \\ &= \lim_{h \to 0} \frac{\mathrm{Im}[f(x + i(y + h))] - \mathrm{Im}[f(x + iy)]}{h} \end{aligned}$$

Note: For real-valued f,

$$y = 0 \; , f(x) = u(x, 0) \; , v(x, 0) = \mathrm{Im}[f(x)] = 0$$

Complex-Step Approximation:

$$f'(x) \approx \frac{\mathrm{Im}[f(x + ih)]}{h}$$

Complex-Step Derivative Approximation

Complex-Step Approximation:

$$f'(x) \approx \frac{\text{Im}[f(x+ih)]}{h}$$

A Bit of History: Discussed in

- J.N. Lyness and C.B. Moler, “Numerical Differentiation of Analytic Functions,” *SIAM Journal on Numerical Analysis*, 4, pp. 202-210, 1967.

Big Problem: Assumption of analyticity overly restrictive for simulation codes

Solution: For sufficiently smooth f, consider

$$f(x+ih) = f(x) + ihf'(x) - \frac{h^2}{2!}f''(x) - i\frac{h^3}{3!}f^{(3)}(x) + \mathcal{O}(h^4)$$

Complex-Step Approximation:

$$f'(x) = \frac{\text{Im}[f(x+ih)]}{h} + \mathcal{O}(h^2)$$

Note:

- Reduces smoothness requirement
- Numerically demonstrated to be accurate up to points of discontinuity

Complex-Step Derivative Approximation

Complex-Step Approximation:

$$f'(x) = \frac{\text{Im}[f(x+ih)]}{h} + \mathcal{O}(h^2)$$

A Bit More History:

- Used to compute sensitivities for 3-D aero-structural models – verified using adjoints: [Martins et al, 2003].
- Noted by Tim Kelley in his green book.
- Employed for delay-differential equations with non-smooth initial functions – verified using sensitivity equations: [Banks et al, 2015].

Notes:

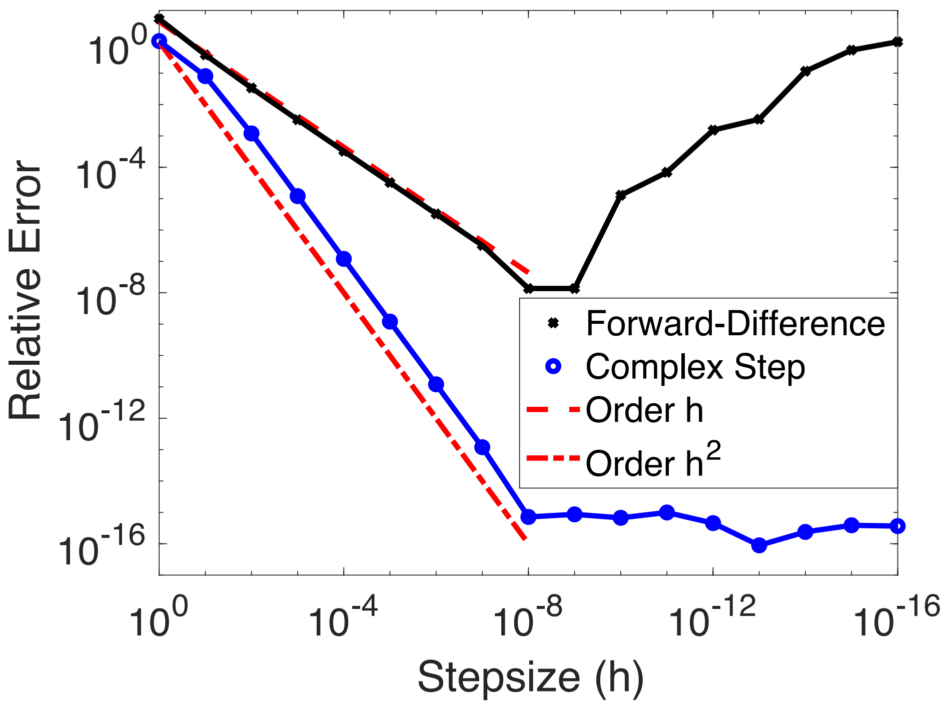
- Avoids subtractive cancellation and relatively insensitive to stepsize.
- May require modification of MATLAB functions such as *abs, min, max*.
- Structure very similar to forward-mode AD.
- Surprisingly robust and difficult to break!

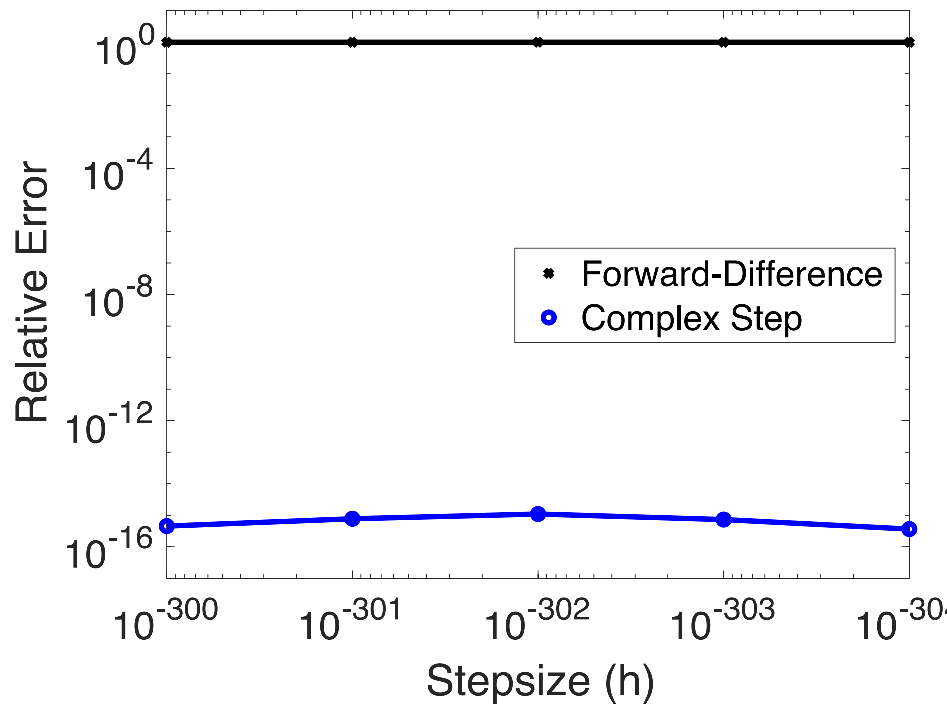
Complex-Step Derivative Approximation

Analytic Example: Based on example in J.N. Lyness and C.B. Moler, 1967.

$$f(x) = \frac{e^{2x}}{\sqrt{\sin^2 x + \cos^2(3x)}}$$

Relative Errors: Complex-step and finite-difference $e_{rel} = \frac{|f' - f'_{exact}|}{|f'_{exact}|}$





Complex-Step Derivative Approximation

Example: 3-parameter SIR model

$$\frac{dS}{dt} = \delta(N - S) - \gamma IS \quad , \quad S(0) = S_0$$

$$\frac{dI}{dt} = \gamma IS - (r + \delta)I \quad , \quad I(0) = I_0,$$

Sensitivity Equations:

$$\frac{ds(t)}{dt} = \frac{\partial g}{\partial u} s(t) + \frac{\partial g}{\partial q}$$

$$s(t_0) = 0_{N \cdot p}$$

$$s(t) = \left[\frac{\partial S}{\partial \delta}, \frac{\partial I}{\partial \delta}, \frac{\partial S}{\partial \gamma}, \frac{\partial I}{\partial \gamma}, \frac{\partial S}{\partial r}, \frac{\partial I}{\partial r} \right]^T$$

$$\frac{\partial g}{\partial u} = \begin{bmatrix} J & 0 & 0 \\ 0 & J & 0 \\ 0 & 0 & J \end{bmatrix} , \; J = \begin{bmatrix} -\delta - \gamma I & -\gamma S \\ \gamma I & \gamma S - (r + \delta) \end{bmatrix}$$

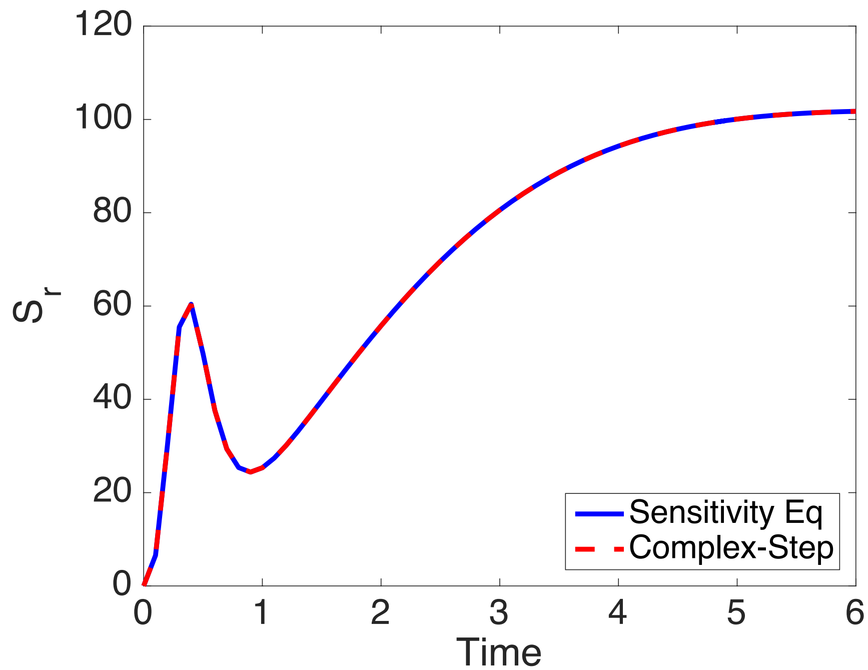
$$\frac{\partial g}{\partial q} = [(N - S), -I, -IS, IS, 0, -I]^T .$$

Complex-Step Derivative Approximation

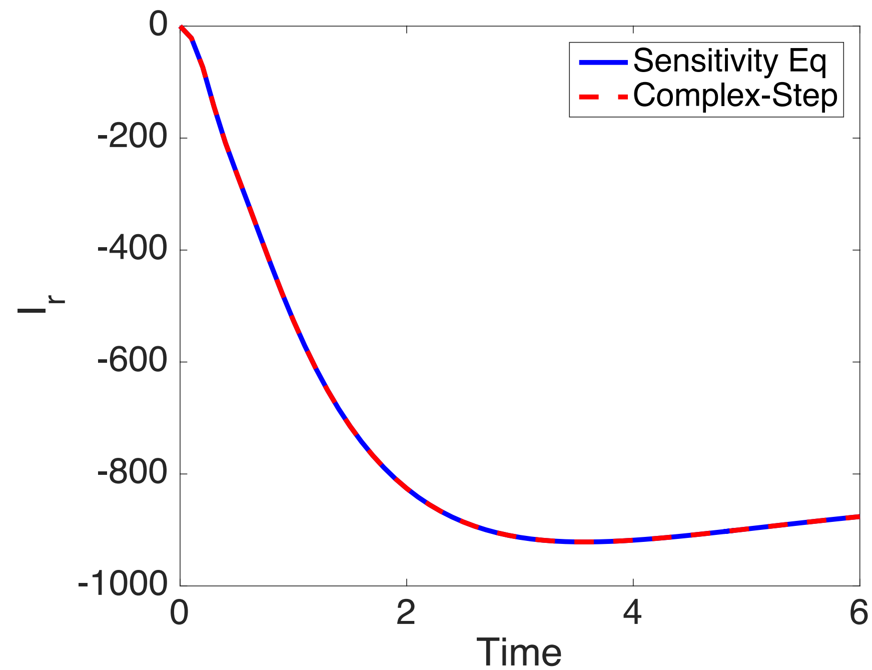
Example: 3-parameter SIR model

$$\frac{dS}{dt} = \delta(N - S) - \gamma IS \quad , \quad S(0) = S_0$$
$$\frac{dI}{dt} = \gamma IS - (r + \delta)I \quad , \quad I(0) = I_0,$$

Results: Representative parameter sensitivities



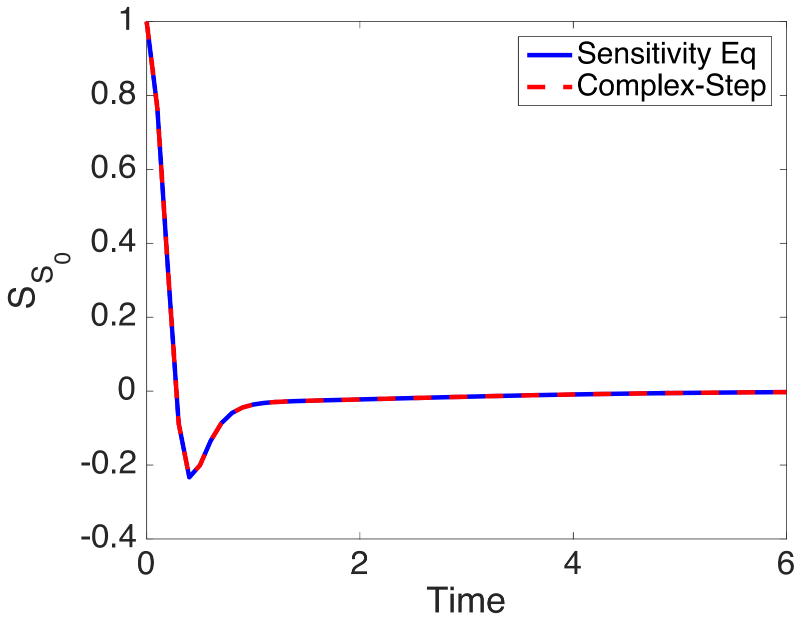
$$\frac{\partial S}{\partial r}(t)$$



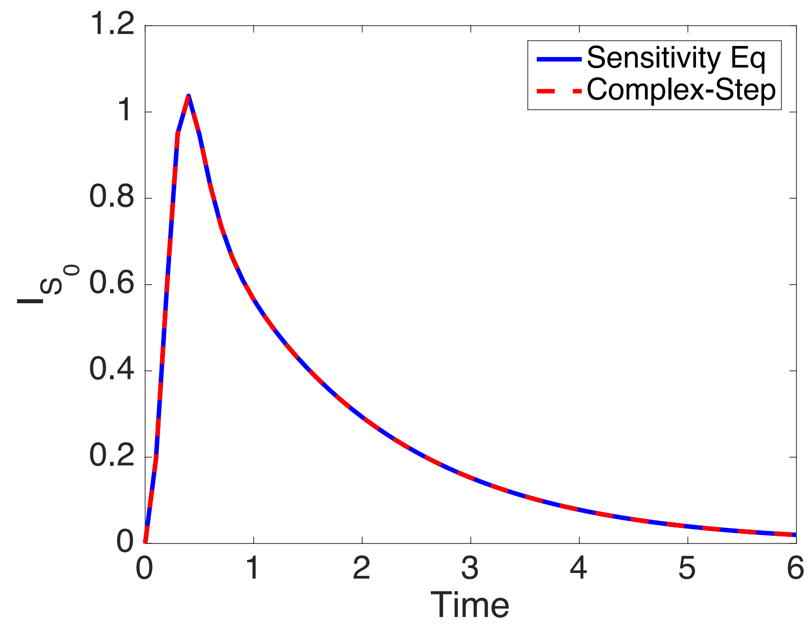
$$\frac{\partial I}{\partial r}(t)$$

Complex-Step Derivative Approximation

Results: Representative initial condition sensitivities



$$\frac{\partial S}{\partial S_0}(t)$$



$$\frac{\partial I}{\partial S_0}(t)$$

Notes:

- Complex-step required modification of two lines of code:

  S0_complex = complex(S0,h); S_S0 = imag(Y(:,1))/h;

- Accuracy dictated by accuracy of ODE solver.
- Significantly easier to code than sensitivity equations!

Complex-Step Derivative Approximation

Euler-Bernoulli Model: 0 < x < L, t > 0

$$\rho(x)\frac{\partial^2 w}{\partial t^2} + \gamma\frac{\partial w}{\partial t} + \frac{\partial^2 M}{\partial x^2} = f(t,x)$$

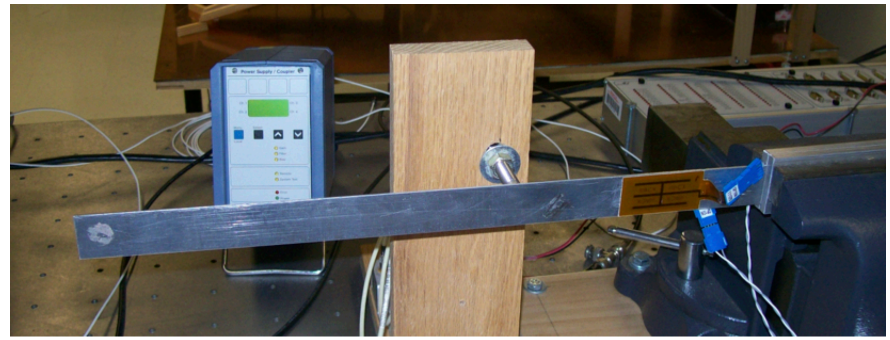
$$M(t,x) = YI(x)\frac{\partial^2 w}{\partial x^2} + cI(x)\frac{\partial^3 w}{\partial x^2 \partial t}$$

Here

$$\rho(x) = \rho hb + \rho_p h_p b_p \chi_p(x),$$

$$YI(x) = YI_b + YI_p \chi_p(x),$$

$$cI(x) = cI_b + cI_p \chi_p(x)$$



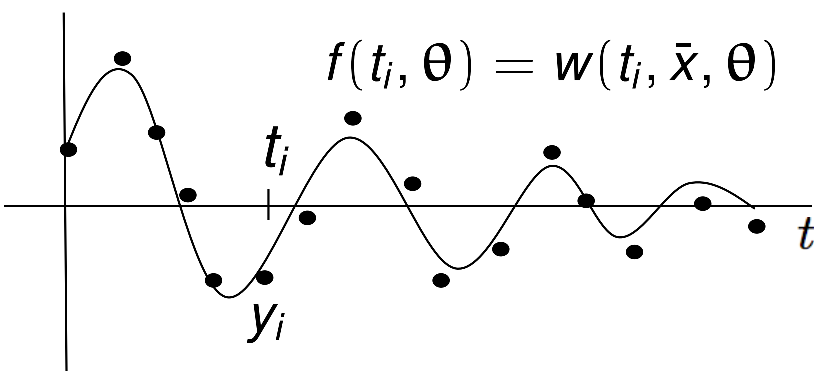
Parameters:

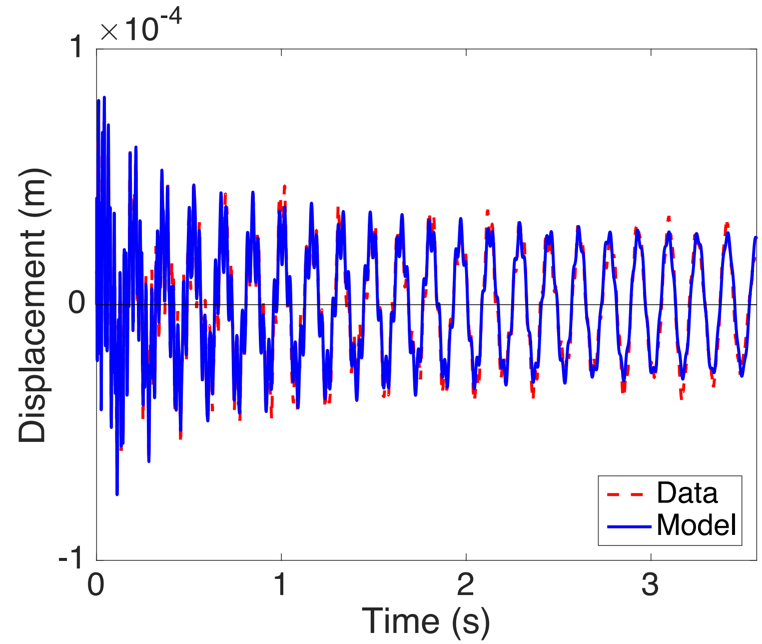
$$\theta = [YI_b, cI_b, \gamma, k_p, \rho_p, YI_p, cI_p]$$

Observation Model:

$$y_i = f(t_i, \theta) + \varepsilon_i$$

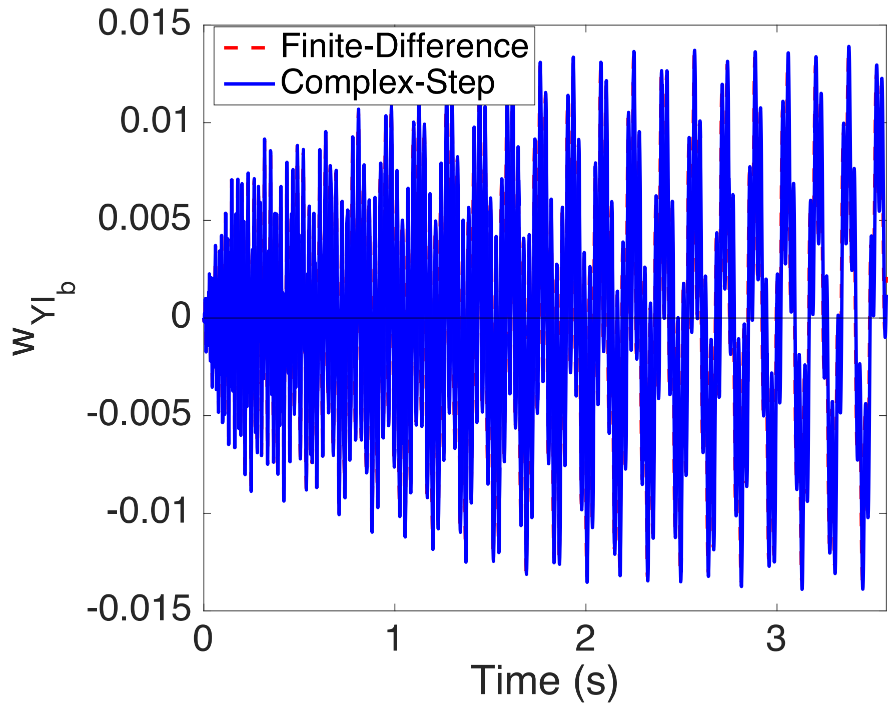
$$f(t_i, \theta) = w(t_i, \bar{x}, \theta)$$

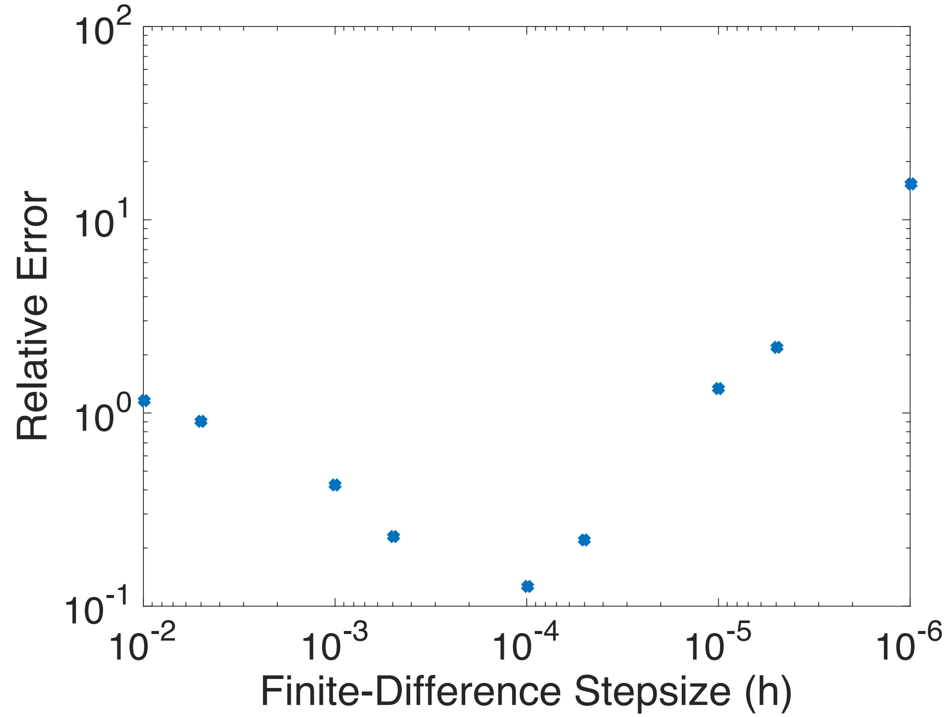




Complex-Step Derivative Approximation

Goal: Approximate $s_{CS}(t) = \frac{\partial w(t)}{\partial YI_b}$ ← Stiffness coefficient





Finite Difference: $h = 1 \times 10^{-4}$

Complex-Step: $h = 1 \times 10^{-16}$

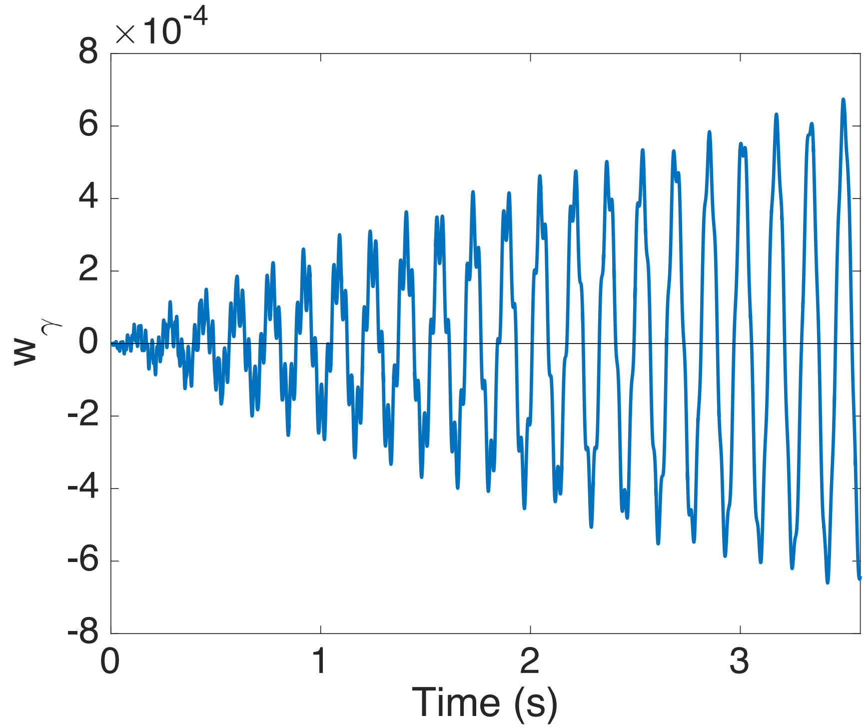
$$e_{rel} = \frac{\max_{t \in [0,T]} |s_{CS}(t) - s_{FD}(t)|}{\max_{t \in [0,T]} |s_{CS}(t)|}$$

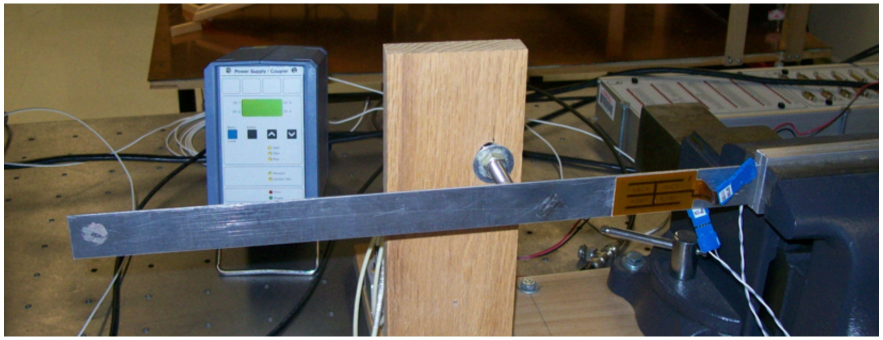
Note:

- Complex-step accuracy relatively insensitive to stepsize.
- Difficult to compute reasonable finite-difference sensitivity.

Complex-Step Derivative Approximation

Goal: Approximate $s_{CS}(t) = \dfrac{\partial w(t)}{\partial \gamma}$ ← Air damping





Notes:

- Most affected by primary mode
- Could not get reasonable approximation using finite-differences

Automatic Differentiation

Approach: Apply chain rule to elementary arithmetic operations and functions

Example: Differentiate $f(x_1, x_2) = x_1 x_2^2$ with respect to x_2

Forward AD	Complex-Step Method
$\Delta x_1 = 0$	$h_1 = 0$
$\Delta x_2 = 1$	$h_2 = 10^{-16}$
$f(x_1, x_2) = x_1 x_2^2$	$f = (x_1 + ih_1)(x_2 + ih_2)^2$
$\Delta f = \Delta x_1 x_2^2 + 2x_1 x_2 \Delta x_2$	$f = [x_1(x_2 - h_2^2) - 2x_2 h_1 h_2]$
	$+i[h_1(x_2^2 - h_2^2) + 2x_1 x_2 h_2]$
$\frac{\partial f}{\partial x_2} = \Delta f = 2x_1 x_2$	$\frac{\partial f}{\partial x_2} = \frac{Im[f]}{h_2} = 2x_1 x_2$

Concluding Remarks

Advantages:

- Easy to code.
- Provides second-order accuracy with one function evaluation and relatively insensitive to stepsize.
- Avoids solving coupled sensitivity equations for evolution models.
- Numerical tests demonstrate accuracy up to discontinuities for several applications.
- Close ties to forward AD but does not require AD architectures.

Disadvantages:

- Can fail without numerical warning for problems with insufficient regularity.
- Requires p model evaluations for p inputs. Can be a problem for high-dimensional problems.
- Requires modification of certain functions such as *abs, min, max*.
- Does not run automatically in MATLAB pde toolbox.