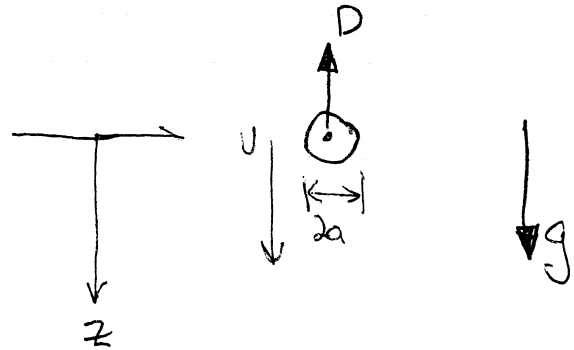


Backward Euler example: Particle in free-fall Feb 15 Notes | 1

Consider a spherical particle falling through the atmosphere:

$$D = \frac{1}{2} \rho_g \pi a^2 u^2 C_D(\text{Re})$$

$$\text{Re} = \frac{\rho_g u 2a}{\mu_g}$$



$$C_D = \frac{24}{\text{Re}} + \frac{6}{1 + \sqrt{\text{Re}}} + 0.4$$

$$\text{at } t=0, \quad z=0, \quad u=0$$

Governing equations:

$$m_p \dot{u} = m_p g - D$$

$$\dot{z} = u$$

So, in our canonical form:

$$\dot{u} = g - \frac{1}{m_p} D = f_u(u)$$

$$\dot{z} = u = f_z(u)$$

Or

$$\dot{\vec{u}} = \vec{F} \quad \text{where } \vec{u} = \begin{bmatrix} u \\ z \end{bmatrix}$$

$$\vec{F} = \begin{bmatrix} g - \frac{1}{m_p} D \\ u \end{bmatrix}$$

As described in the previous notes, we need $\frac{\partial \vec{F}}{\partial \vec{u}}$. ~~Here is that.~~ To do this, I

would strongly recommend using the chain rule to keep this clean.

$$\text{First, } f_0 = g - \frac{1}{m_p} D$$

Note, f_0 does not depend on z

$$\Rightarrow \boxed{\frac{\partial f_0}{\partial z} = 0}$$

The harder one is $\frac{\partial f_0}{\partial U}$

$$\frac{\partial f_0}{\partial U} = \frac{\partial}{\partial U} \left(g - \frac{1}{m_p} D \right)$$

$$\boxed{\frac{\partial f_0}{\partial U} = -\frac{1}{m_p} \frac{\partial D}{\partial U}}$$

$$D = \frac{1}{2} \rho g \pi a^2 U^2 C_D(\text{Re})$$

$$\Rightarrow \frac{\partial D}{\partial U} = \frac{1}{2} \rho g \pi a^2 U^2 \frac{\partial C_D}{\partial \text{Re}} \frac{\partial \text{Re}}{\partial U} + \frac{1}{2} \rho g \pi a^2 (2U) C_D(\text{Re})$$

$$\frac{\partial \text{Re}}{\partial U} = \frac{\partial}{\partial U} \left(\frac{\rho U 2a}{\mu g} \right) = \frac{2a \rho g}{\mu g}$$

$$\frac{\partial C_D}{\partial \text{Re}} = \frac{\partial}{\partial \text{Re}} \left[\frac{24}{\text{Re}} + \frac{6}{1 + \sqrt{\text{Re}}} + 0.4 \right] = -\frac{24}{\text{Re}^2} - 6(1 + \sqrt{\text{Re}})^{-2} \frac{1}{2} \text{Re}^{-\frac{1}{2}}$$

$$\text{Then } f_z = U \Rightarrow \frac{\partial f_z}{\partial z} = 0 \quad \frac{\partial f_z}{\partial U} = 1$$

$$\Rightarrow \frac{\partial f}{\partial U} = \begin{bmatrix} -\frac{1}{m_p} \frac{\partial D}{\partial U} & 0 \\ 1 & 0 \end{bmatrix}$$

In some case, calculation of the derivatives $\frac{\partial f_0}{\partial u}$ may be extremely difficult to do by hand even with careful chain rule application.

In that case, finite differencing may be used to find these derivatives:

For example,

$$\left. \frac{\partial f_0}{\partial u} \right|_{FD} = \frac{f_0(u+\epsilon) - f_0(u-\epsilon)}{2\epsilon} = \frac{\partial f_0}{\partial u} + O(\epsilon^2)$$

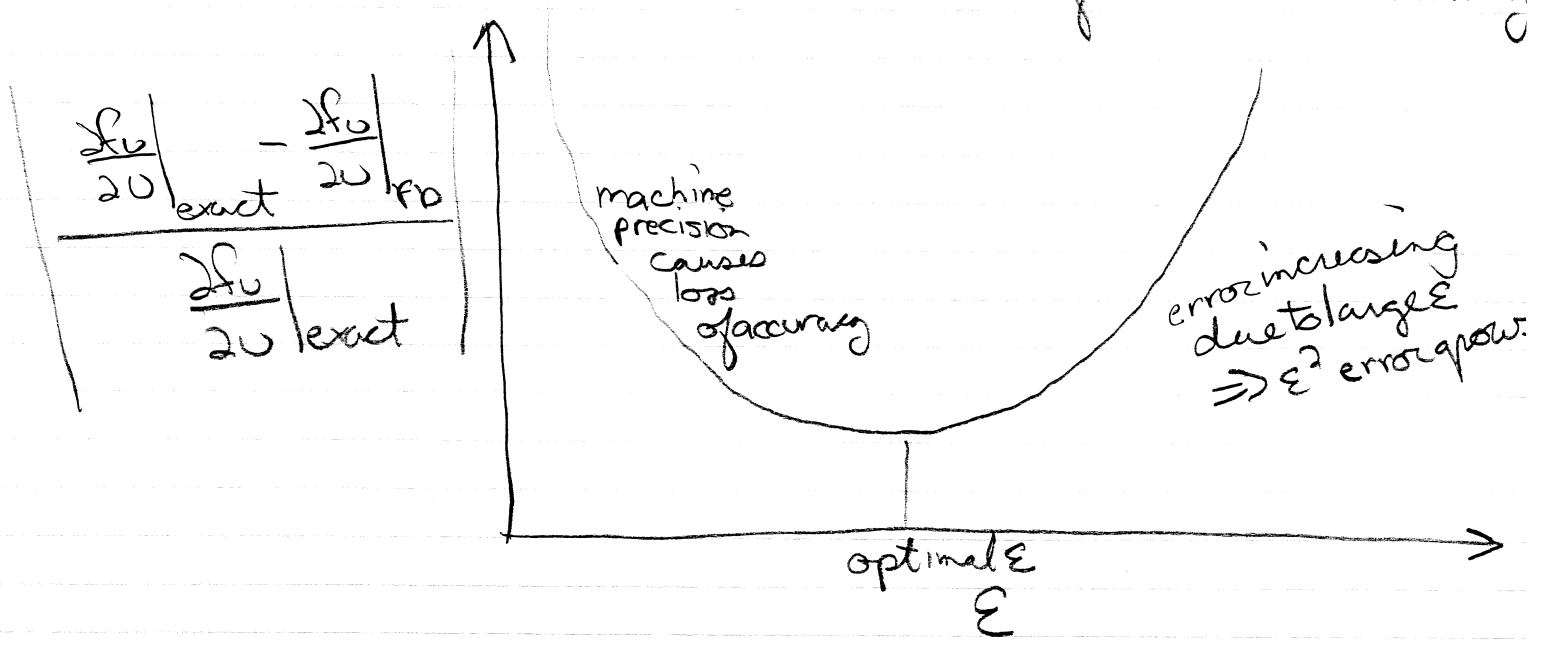
error
↓

where ϵ is a small number typically $\epsilon \approx 1 \times 10^{-6}$

Warning: There is some judgement in choosing ϵ .

* If taken too large, the derivative will not be accurate.

* If taken too small, the precision of the computer will be run into and the derivatives will again lose accuracy.



Typically, the optimal ϵ is around
 $\epsilon_{opt} \approx \sqrt{\text{Machine precision}}$.

Comments on using finite differences $\frac{\partial \vec{F}}{\partial \vec{v}}$:

- * Very useful for debugging! If $\vec{F}(\vec{v}, t)$ is difficult to differentiate, then comparing $\left. \frac{\partial \vec{F}}{\partial \vec{v}} \right|_{FD}$ and a hand-coded $\frac{\partial \vec{F}}{\partial \vec{v}}$ is an essential tool.
- * Finite differences are usually (though not always) slower than hand-coded derivatives. Though, with careful implementation of finite differences, the cost is usually only 3-4 times hand-coding.
- * If you are using a blackbox integrator (such as in matlab), the differentiation will be done w/ finite differences, but, usually the user can supply the derivatives if desired.

```
clear all;

% Initialize some parameters
rhog = 0.9; % Density of air at 3000m
a = 0.01; % Particle radius
mu = 1.693e-5; % Viscosity of air at 3000m
g = 9.8; % Gravity
mp = 917*4*pi/3*a^3; % mass of ice particle

% Initial conditions
u0 = 0.001; % Use a small initial velocity to avoid problems with Re=0 and CD
z0 = 0; % Initial particle location

% Set time length of integration, and number of steps
Tmax = 25;
N = 100;
dt = Tmax/N;

f = zeros(2,1);
v(:,1) = [u0; z0];
% Start iterative loop
for n = 2:N+1,

% Calculate drag at n-1
u = v(1,n-1);
Re = rhog*u*(2*a)/mu;
CD = 24/Re + 6/(1+sqrt(Re)) + 0.4;
D = 0.5*rhog*u^2*pi*a^2*CD;

% Calculate right-hand sides at n-1
f(1) = g - D/mp;
f(2) = u;

% Update using Forward Euler
v(:,n) = v(:,n-1) + dt*f;

end

% Plot results
t = linspace(0,Tmax,N+1);
u = v(1,:);
z = v(2,:);

subplot(211);
plot(t,z);
xlabel('time');ylabel('z');
title('Forward Euler integration');

subplot(212);
plot(t,u);
xlabel('time');ylabel('u');
```

```

clear all;

% Initialize some parameters
rhog = 0.9; % Density of air at 3000m
a = 0.01; % Particle radius
mu = 1.693e-5; % Viscosity of air at 3000m
g = 9.8; % Gravity
mp = 917*4*pi/3*a^3; % mass of ice particle

% Initial conditions
u0 = 0.001; % Use a small initial velocity to avoid problems with Re=0 and CD
z0 = 0; % Initial particle location

% Set time length of integration, and number of steps
Tmax = 25;
N = 100;
dt = Tmax/N;

% Set Newton-Raphson convergence parameters
Mmax = 10;
restol = 1e-4;

% Initialize vector for ODE integration
f = zeros(2,1);
w = zeros(2,1);
res = zeros(2,1);
v(:,1) = [u0; z0];

% Start iterative loop
for n = 2:N+1,

% Begin sub-iteration loop
m = 0;
curren = restol + 1; % Doing this forces at least one sub-iteration to occur
w = v(:,n-1);
while ((m < Mmax) & (curren > restol)),

    u = w(1);
    Re = rhog*u*(2*a)/mu;
    pRe_pu = rhog*(2*a)/mu;

    CD = 24/Re + 6/(1+sqrt(Re)) + 0.4;
    pCD_pRe = -24*Re^(-2) - 6*(1+sqrt(Re))^(-2)*0.5/sqrt(Re);

    D = 0.5*rhog*u^2*pi*a^2*CD;
    pD_pu = 0.5*rhog*u^2*pi*a^2*pCD_pRe*pRe_pu + rhog*pi*a^2*u*CD;

% Calculate right-hand sides using w
f(1) = g - D/mp;
f(2) = u;

% Calculate residual
res = w - v(:,n-1) - dt*f;
curren = norm(res);

% Calculate linearization of f with respect to w
pf_pw(1,1) = -pD_pu/mp; % this is pfu/pu
pf_pw(1,2) = 0.0; % this is pfu/pz
pf_pw(2,1) = 1.0; % this is pfz/pu
pf_pw(2,2) = 0.0; % this is pfz/pz

% Calculate linearization of residual with respect to w
pres_pw = eye(size(pf_pw)) - dt*pf_pw;

% Calculate dw from pres_dw*dw = -res
dw = -pres_pw\res;
w = w + dw;

```

```

% Increment sub-iteration counter
m = m + 1;

end

% Check on convergence and update states
if (curren > restol),
    fprintf('Maximum number of Newton sub-iterations occurred\n');
end

v(:,n) = w;

end

% Plot results
t = linspace(0,Tmax,N+1);
u = v(1,:);
z = v(2,:);

subplot(211);
plot(t,z);
xlabel('time');ylabel('z');
title('Backward Euler integration');

subplot(212);
plot(t,u);
xlabel('time');ylabel('u');

```

```

clear all;

% Initialize some parameters
rhog = 0.9; % Density of air at 3000m
a = 0.01; % Particle radius
mu = 1.693e-5; % Viscosity of air at 3000m
g = 9.8; % Gravity
mp = 917*4*pi/3*a^3; % mass of ice particle

% Store the parameters in a vector for later use
p = [rhog, a, mu, g, mp];

% Initial conditions
u0 = 0.001; % Use a small initial velocity to avoid problems with Re=0 and CD
z0 = 0; % Initial particle location

% Set time length of integration, and number of steps
Tmax = 25;
N = 100;
dt = Tmax/N;
eps = 1e-4; % Finite difference step size for pf_pw calculation

% Set Newton-Raphson convergence parameters
Mmax = 10;
restol = 1e-4;

% Initialize vector for ODE integration
f = zeros(2,1);
w = zeros(2,1);
res = zeros(2,1);
v(:,1) = [u0; z0];

% Start iterative loop
for n = 2:N+1,

% Begin sub-iteration loop
m = 0;
curre = restol + 1; % Doing this forces at least one sub-iteration to occur
w = v(:,n-1);
while ((m < Mmax) & (curre > restol)),

% Calculate rhs
f = drop_rhs(w, p);

% Calculate residual
res = w - v(:,n-1) - dt*f;
curre = norm(res);

% Calculate linearization of f with respect to w using finite differences
for ii = 1:2,
w0 = w(ii);

w(ii) = w0 + eps; % Perturb ii state by eps
fp = drop_rhs(w, p);

w(ii) = w0 - eps; % Perturb ii state by -eps
fm = drop_rhs(w, p);

w(ii) = w0; % Restore ii state to original value

pf_pw(:,ii) = (fp - fm)/(2*eps); % Finite difference
end

% Calculate linearization of residual with respect to w
pres_pw = eye(size(pf_pw)) - dt*pf_pw;

% Calculate dw from pres_dw*dw = -res

```

```

dw = -pres_pw\res;
w = w + dw;

% Increment sub-iteration counter
m = m + 1;

end

% Check on convergence and update states
if (curre > restol),
fprintf('Maximum number of Newton sub-iterations occurred\n');
end

v(:,n) = w;

end

% Plot results
t = linspace(0,Tmax,N+1);
u = v(1,:);
z = v(2,:);

subplot(211);
plot(t,z);
xlabel('time');ylabel('z');
title('Backward Euler integration with finite-differenced pf/pw');

subplot(212);
plot(t,u);
xlabel('time');ylabel('u');

```

```
function [f] = drop_rhs(w, p)
```

```
% Returns rhs of particle equation given the current state (w)  
% and the parameters of the problem (p)
```

```
% Unpack the parameters from p
```

```
rhog = p(1);  
a     = p(2);  
mu    = p(3);  
g     = p(4);  
mp    = p(5);
```

```
% Get velocity
```

```
u = w(1);
```

```
% Calculate drag
```

```
Re = rhog*u*(2*a)/mu;  
CD = 24/Re + 6/(1+sqrt(Re)) + 0.4;  
D = 0.5*rhog*u^2*pi*a^2*CD;
```

```
% Calculate right-hand sides
```

```
f = zeros(2,1);  
f(1) = g - D/mp;  
f(2) = u;
```