Discretization of the Advection-Diffusion Equation

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clear, clc, close all
set_demo_defaults
```

Consider the Advection-Diffusion Equations (ADE) for the heat transport by advection and conduction

$$\frac{\partial T}{\partial t} + \nabla \cdot (\mathbf{v}T - k\nabla T) = f_s$$

where we have assumed that ρ and c_p are constant and divided by them, so that $k = \kappa/(\rho c_p)$ is the thermal diffusivity. Using the θ-method and our discrete operators we discretize this equation as follows

$$\mathbf{I}\frac{\mathbf{u}^{n+1} - \mathbf{u}^n}{\Delta t} + \mathbf{D} * (\mathbf{A}(\mathbf{v}) - \mathbf{Kd} * \mathbf{G}) * (\theta \mathbf{u}^{n+1} + (1-\theta)\mathbf{u}^{n+1}) = \mathbf{f}_s$$

Here both the advective and diffusive/conductive terms are treated equally. Let's first consider the purely advective case, $k = 0$ and $f_s = 0$, so that

$$\mathbf{IM} * \mathbf{u}^{n+1} = \mathbf{EX} * \mathbf{u}^n$$

where implicit and explicit matrices are given by

$$\mathbf{IM} = \mathbf{I} + \Delta t(1-\theta)\mathbf{D} * \mathbf{A}(\mathbf{v})$$

$$\mathbf{EX} = \mathbf{I} - \Delta t\,\theta\,\mathbf{D} * \mathbf{A}(\mathbf{v})$$

here $\mathbf{A}(\mathbf{v})$ is the matrix that computes the upwind flux based on the sign of $\mathbf{v}$.

```
v0= 1;
Grid.xmin = 0; Grid.xmax = 1; Grid.Nx = 30;
Grid.periodic = 'x-dir';
Grid = build_grid(Grid);
[D,G,~,I,M] = build_ops(Grid);
v = v0*ones(Grid.Nfx,1); A = flux_upwind(v,Grid);
L = D*A; S = I;
IM = @(theta,dt) S + (1-theta)*dt*L;
EX = @(theta,dt) S - theta*dt*L;
```

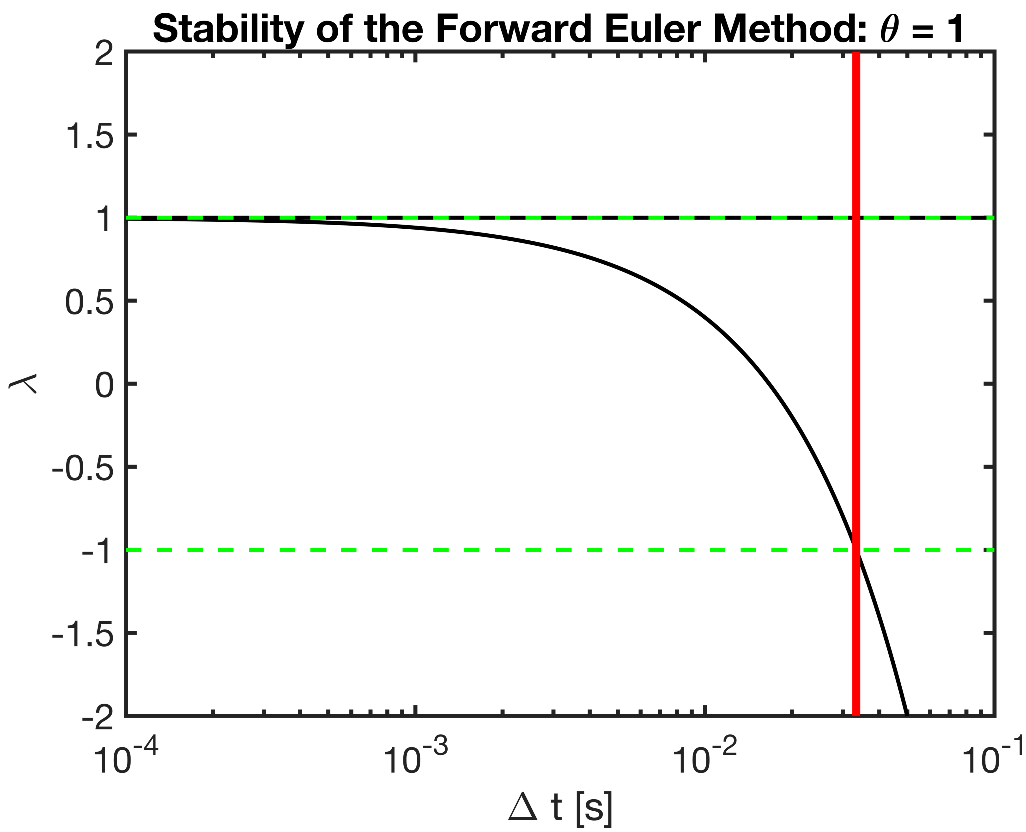
Explicit advective time step restriction (CFL-condition)

Similar to the diffusive case the Forward Euler Method ($\theta = 1$) is only conditionally stable. Again we can confirm this by looking at the eigenvalue spectrum of the resulting amplification matrix, $\mathbf{AMP} = \mathbf{IM}^{-1}\mathbf{EX}$. For an advection problem we cannot impose natural boundary conditions, hence we impose periodic BC's - something we have not discussed in class (but not very difficult).

```
theta = 1;
dt_max = Grid.dx/(v0);
dt_vec = logspace(-4,-1,3e2);

figure
```

```
for i = 1:length(dt_vec)
    A = inv(IM(theta,dt_vec(i)))*EX(theta,dt_vec(i));
    lam = eig(full(A));
    lam_max_FE(i) = max(lam);
    lam_min_FE(i) = min(lam);
end
semilogx(dt_vec,lam_max_FE,'k'), hold on
semilogx(dt_vec,lam_min_FE,'k')
semilogx(dt_vec,ones(size(dt_vec)),'g--','linewidth',2)
semilogx(dt_vec,-ones(size(dt_vec)),'g--','linewidth',2)
semilogx(dt_max*[1 1],[-2 2],'r','linewidth',4), hold off
ylim([-2 2])
xlabel '\Delta t [s]'
ylabel('\lambda')
title 'Stability of the Forward Euler Method: \theta = 1'
```



For $\Delta t > \Delta x/|v|$ the magnitude of the largest eigenvalues exceeds 1 and the method is unstable (red line). This criterion is referred to a the Courant-Friedrichs-Levy condtion or CFL-condition.

Comparison to Neumann condtion for diffusion

It is worth comparing the explicit time step limits for both diffusion and advection as function of the dimensionless grid size, $\Delta x' = \Delta x/L$, and the Peclet number, $Pe = vL/k$, where L is the domain size. Given the two conditions on the time step $\Delta t_N \leq \Delta x^2/(2k)$ and $\Delta t_{\text{CFL}} \leq \Delta x/|v|$ we have the ratio

$$\frac{\Delta t_{\text{CFL}}}{\Delta t_{\text{Neu}}} = \frac{2}{\Delta x' Pe}$$

so that the explicit timestep is limited by diffusion when $\Delta x' < 2/\text{Pe}$. Therefore, as the grid is refined the time step is always limited by diffusion. In fluid dynamical problems surch as convection in the ice shell, $\mathbf{Pe} \gg 1$, so that advection may limit the time step for realistic problems with finite grid size.

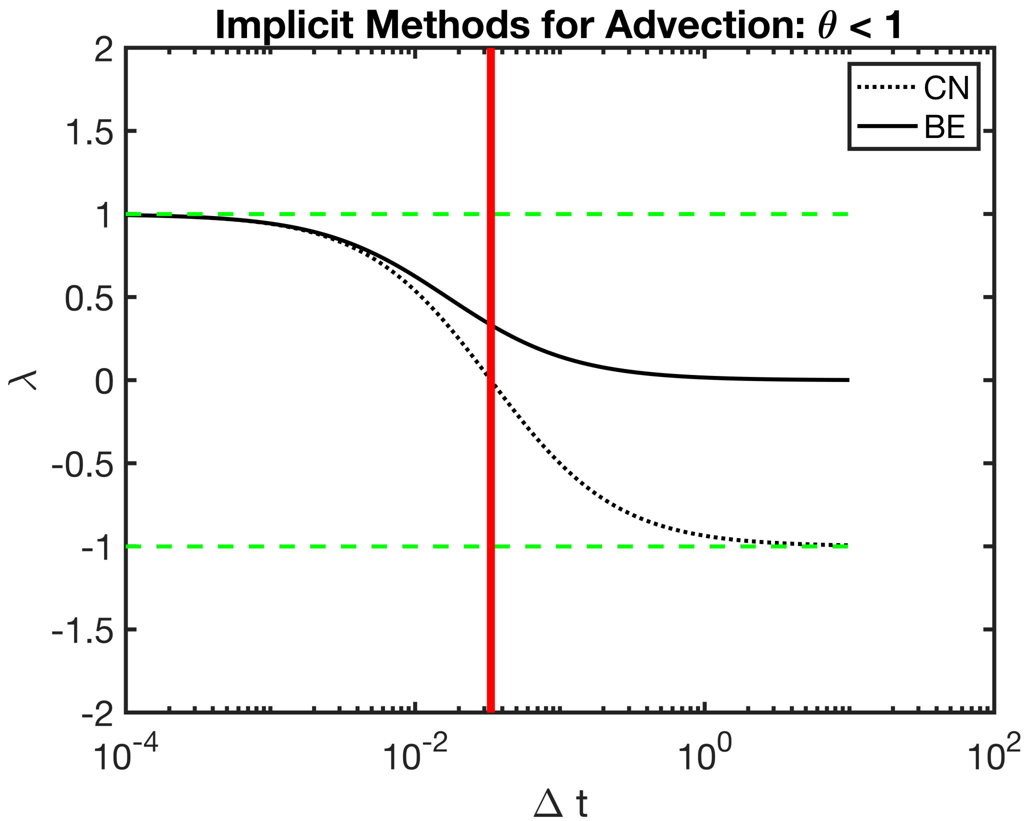
Implicit advective time stepping

Of course, we can also choose the implicit Backward Euler (BE) and Crank-Nicholson Methods (CN) to time step the advection equation.

```
theta = 1;
dt_max = Grid.dx/(v0);
dt_vec = logspace(-4,1,3e2);
lam_max_BE = zeros(length(dt_vec),1);
lam_max_CN = lam_max_BE;
lam_min_BE = lam_max_BE;
lam_min_CN = lam_max_BE;

figure
for i = 1:length(dt_vec)
    theta = 0; % BE
    A = inv(IM(theta,dt_vec(i)))*EX(theta,dt_vec(i));
    lam = eig(full(A));
    lam_max_BE(i) = max(lam);
    lam_min_BE(i) = min(lam);

    theta = 0.5; % CN
    A = inv(IM(theta,dt_vec(i)))*EX(theta,dt_vec(i));
    lam = eig(full(A));
    lam_max_CN(i) = max(lam);
    lam_min_CN(i) = min(lam);
end
semilogx(dt_vec,lam_min_CN,'k:'), hold on
semilogx(dt_vec,lam_min_BE,'k')
semilogx(dt_vec,ones(size(dt_vec)),'g--','linewidth',2)
semilogx(dt_vec,-ones(size(dt_vec)),'g--','linewidth',2)
semilogx(dt_max*[1 1],[-2 2],'r','linewidth',4), hold off
ylim([-2 2])
xlabel '\Delta t'
ylabel('\lambda')
title 'Implicit Methods for Advection: \theta < 1'
legend('CN','BE')
```



Transient solution

```
theta = 1;   Nx = 100; Length = 2;  v0 = 1; phi =1;
tmax = 1.5; cfl = .5;

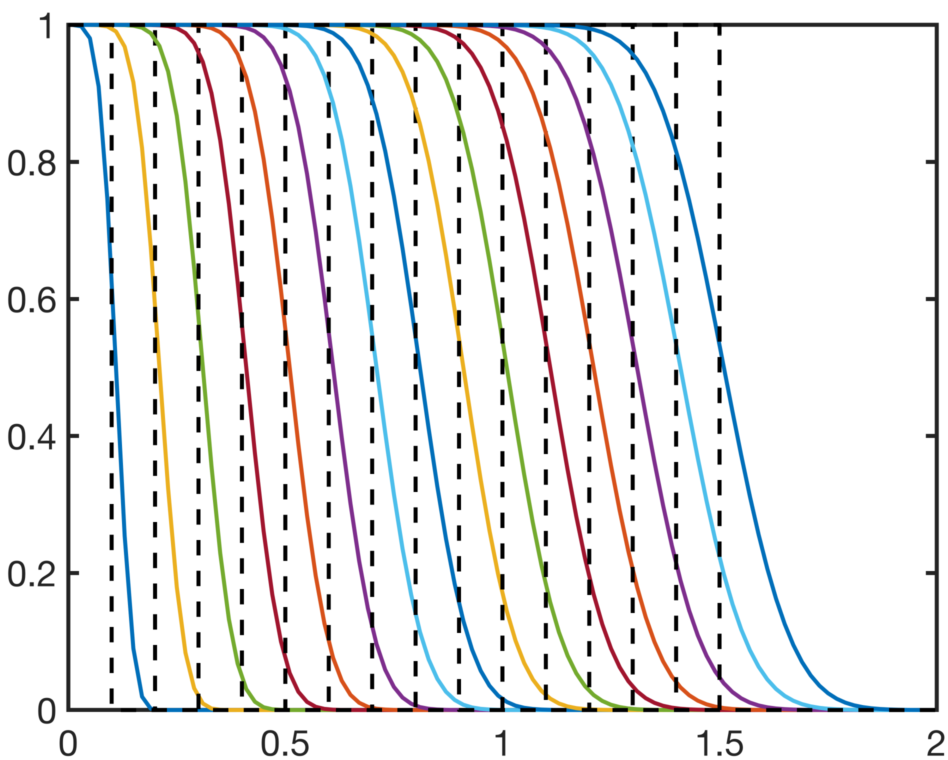

% Grid and operators
Grid.xmin = 0; Grid.xmax = Length; Grid.Nx = Nx;
Grid = build_grid(Grid);
[D,G,~,I,M] = build_ops(Grid);
dt = cfl*Grid.dx/(v0);
Nt = round(tmax/dt);
v = v0*ones(Grid.Nfx,1);
A = flux_upwind(v,Grid);

% Assemble implicit and explicit operators
IM = @(theta)  I + (1-theta)*dt/phi*(D*A);
EX = @(theta)  I - theta*dt/phi*(D*A);

% Boundary conditions
BC.dof_dir   = Grid.dof_xmin;
BC.dof_f_dir = Grid.dof_f_xmin;
BC.dof_neu   = [];
BC.dof_f_neu = [];
BC.qb        = [];
BC.g         = 1;
[B,N,fn] = build_bnd(BC,Grid,I);
```

```
% Initial conditions
cFE = zeros(Grid.Nx,1);

% Transient solution
figure
time = 0;
for i=1:Nt
    time = time + dt; xf = v0*time;
    %% Finite Volume
    cFE = solve_lbvp(IM(theta),EX(theta)*cFE,B,BC.g,N);
    if mod(i,10) == 0
    plot(Grid.xc,cFE,'-'), hold on
    plot([0 xf xf Grid.xmax],[1 1 0 0],'k--')
    drawnow
    end
end
```



Numerical diffusion

The main challence in numerical simulation of advective transport is the elimination of so-called numerical diffusion. The numerical example below illustrates this

```
theta = 1;   Nx = 100; Length = 2;  v0 = 1; phi =1;
tmax = .5; cfl = .1;
```

```
% Grid and operators
Grid.xmin = 0; Grid.xmax = Length; Grid.Nx = Nx;
Grid = build_grid(Grid);
[D,G,~,I,M] = build_ops(Grid);
dt = cfl*Grid.dx/(v0);
Nt = round(tmax/dt);
v = v0*ones(Grid.Nfx,1);
A = flux_upwind(v,Grid);

% Assemble implicit and explicit operators
Lim = @(theta)  I + (1-theta)*dt/phi*(D*A);
Lex = @(theta)  I - theta*dt/phi*(D*A);

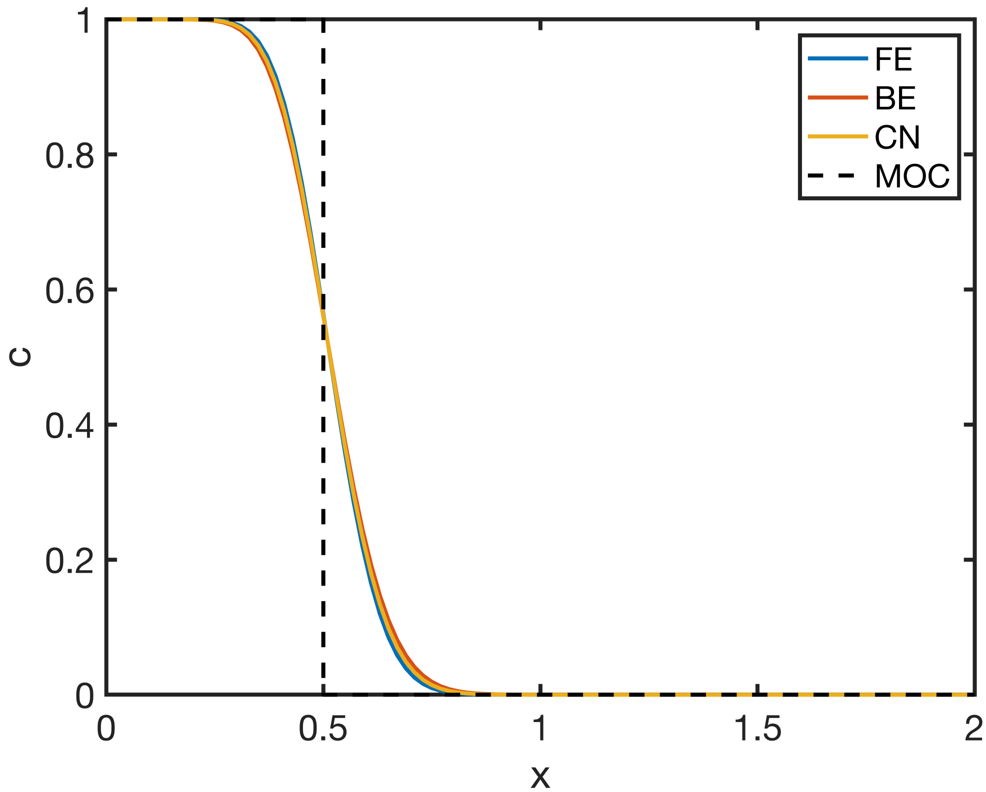
% Boundary conditions
BC.dof_dir   = Grid.dof_xmin;
BC.dof_f_dir = Grid.dof_f_xmin;
BC.dof_neu   = [];
BC.dof_f_neu = [];
BC.qb        = [];
BC.g         = 1;
[B,N,fn] = build_bnd(BC,Grid,I);

% Initial conditions
cFE = zeros(Grid.Nx,1);
cCN = zeros(Grid.Nx,1);
cBE = zeros(Grid.Nx,1);

% Transient solution
figure
time = 0
```

```
time = 0
```

```
for i=1:Nt
    time = time + dt;
    %% Finite Volume
    cFE = solve_lbvp(Lim(1.0),Lex(1.0)*cFE,B,BC.g,N);
    cCN = solve_lbvp(Lim(0.5),Lex(0.5)*cCN,B,BC.g,N);
    cBE = solve_lbvp(Lim(0.0),Lex(0.0)*cBE,B,BC.g,N);
end
xf = v0*time;
clf
plot(Grid.xc,cFE,'-'), hold on
plot(Grid.xc,cBE,'-')
plot(Grid.xc,cCN,'-')
plot([0 xf xf Grid.xmax],[1 1 0 0],'k--')
xlabel 'x'
ylabel 'c'
legend('FE','BE','CN','MOC')
```



Auxillary functions

Advection-diffusion front

This function evaluates the analytic solution for an advection dffusion front in a semi-infinte half space. This solution matches the constant Dirichlet BC at x=0;

```
function [u] = ADEfront(x,t,Pe)
u_lowPe = .5*erfc(sqrt(Pe)*(x-t)/2/sqrt(t)) + ...
           .5*erfc(sqrt(Pe)*(x+t)/2/sqrt(t)).*exp(Pe*x);
u_highPe = .5*         erfc(sqrt(Pe)*(x-t)/2/sqrt(t));

% eliminate nan's and inf's from
switch_vec = isnan(u_lowPe) + isinf(u_lowPe);
u_highPe(switch_vec==0) = 0;
u_lowPe( switch_vec==1) = 0;

u = u_lowPe + u_highPe;
end
```