## Forward testing of differentiation matrices

Note: You will only be able to run this once you have written the functions bulid_grid() and build_ops()!
The discrete operators $\mathbf{D}$ and $\mathbf{G}$ are differentiation matrices. If f is a vector that is the discrete representation of a function $f(x)$, then $\mathbf{G} * \mathbf{f}$ returns a discrete approximation of the derivative $\frac{\partial f}{\partial x}$.

For the one-dimensional examples below the discrete operators can be generated as follows:

```
clear, clc
set_demo_defaults
Grid.xmin = 0; Grid.xmax = 3; Grid.Nx = 10;
Grid = build_grid(Grid);
[D,G,C,I,M] = build_ops(Grid); L = D*G;
```

Here Grid is a structure that contains all information about the grid and build_grid() is a function that generates all the necessary information. The function build_ops () then generates the discrete operators for the grid. The matrix $L$ corresponds to the Laplacian operator and hence to a decond derivative matrix in 1D.

The other matrices returned by build_ops() are:
C = discrete curl (does not exist in 1D)
I = identity
$\mathbf{M}=$ mean matrix - computes arithmetic mean of cell centered values on the cell faces

## Visualizing the fill pattern of the operators

We can viualize the sparity pattern of our matrices with the spy() function.

```
figure(1)
subplot 131
spy(D)
title 'Divergence'
subplot 132
spy(G)
title 'Gradient'
subplot 133
spy(L)
title 'Laplacian'
```



Not the Laplacian has the standard tri-diagonal structure expected for the 1D discretization of the second derivative.

## Testing the discrete operators

We would like to setablish that our discrete operators are correct, before moving on in our implementation. The obvious idea is to solve a particular boundary value problem (BVP) with a known analytic solution and to compare it with the numerical solution. However, this is not the optimal testing strategy, because the full numerical solution of a boundary value problem (BVP) requires both the discrete operators and the implementation of the boundary conditions. The BVP solution may be wrong, even is the diecrete operatores are correct, becuse the error might be in the implementation of boundary condition.

To test only the correctness of the discrete operators, we can use the knowledge that they simply differentiate a function. The only caveat is that the derivative is not evaluated at a the same location, due to the staggered grid!

To test the operators we need a finer grid.

```
Grid.xmin = 0; Grid.xmax = 3; Grid.Nx = 30;
Grid = build_grid(Grid);
[D,G,C,I,M] = build_ops(Grid); L = D*G;
```


## Differentiating a function that statisfies the natural BC's

Consider the function $f(x)=e^{\cos (2 \pi x)}$ on the domain $x \in[0,3]$, which statifies the natural boundary conditions, i.e., $\mathrm{d} f / \mathrm{d} x=0$ at the boundaries. These are the boundary conditions that are build into the discrete gradient G .

```
xa = linspace(Grid.xmin,Grid.xmax,3e2);
f = @(x) exp(cos(2*pi*x));
dfdx = @(x) -exp(cos(2*pi*x)).*sin(2*pi*x)*2*pi;
d2fdx2 = @(x) -2*pi^2*exp(cos(2*pi*x)).*(2*\operatorname{cos}(2*pi*x)+\operatorname{cos}(4*pi*x)-1);
figure(2)
subplot 311
plot(xa,f(xa),'r',Grid.xc,f(Grid.xc),'bo','markerfacecolor','w','markersize'
,6)
xlabel 'x'
ylabel 'f'
legend('analytical','numerical')
subplot 312
plot(xa,dfdx(xa),'r',Grid.xf,G*f(Grid.xc),'bo','markerfacecolor','w','marker
size',6)
xlabel 'x'
ylabel 'df/dx'
legend('analytical','numerical')
subplot 313
plot(xa,d2fdx2(xa),'r',Grid.xc,L*f(Grid.xc),'bo','markerfacecolor','w','mark
ersize',6)
xlabel 'x'
ylabel 'd^2f/dx^2'
legend('analytical','numerical')
```



The figure shows that discrete derivatives approximat the analytic derivatives well. Note that the two derivatives are evaluated at different locations:

1. First derivative is evaluated at cell faces.
2. Second derivative is evaluated at cell centers.

## Differentiation a function that does NOT satisfy the natural BC's

Consider the function $g(x)=e^{\cos (2 \pi x)}$, which does not satify the natural boundary conditions, i.e., the homogeneous Neumann boundary conditions of the discrete gradient operator G .

```
g = @(x) exp(sin(2*pi*x));
dgdx = @(x) exp(sin(2*pi*x)).*cos(2*pi*x)*2*pi;
d2gdx2 = @(x) 2*pi^2*exp(sin(2*pi*x)).*(-2*sin(2*pi*x)+cos(4*pi*x)+1);
```


## figure(3)

subplot 311
plot(xa,g(xa),'r',Grid.xc,g(Grid.xc),'bo','markerfacecolor','w','markersize' ,6)
xlabel 'x'
ylabel 'g'
legend('analytical','numerical')
subplot 312

```
plot(xa,dgdx(xa),'r',Grid.xf,G*g(Grid.xc),'bo','markerfacecolor','w','marker
size',6)
xlabel 'x'
ylabel 'dg/dx'
legend('analytical','numerical')
subplot 313
plot(xa,d2gdx2(xa),'r',Grid.xc,L*g(Grid.xc),'bo','markerfacecolor','w','mark
ersize',6)
xlabel 'x'
ylabel 'd^2g/dx^2'
legend('analytical','numerical')
```



The figure shows that the derivatives are still well approximated in the interior of the domain. The error on the boundaries is large and does not reduce with increasing refinement of the grid. We will see later that the implementation of the boundary condition takes care of this problem.

## Convergence with refinement

To check the convergence of the discrete operators compute the error between $\partial f / \partial x$ and $\mathrm{G} * \mathrm{f}$ and $\partial^{2} f / \partial x^{2}$ and $\mathrm{D} * \mathrm{G} * \mathrm{f}$ as the number grid points increases.

```
Nx = round(logspace(1,6,10));
error_grad = zeros(size(Nx)); error_lap = zeros(size(Nx));
for i = 1:length(Nx)
```

```
    Grid.Nx = Nx(i); Grid = build_grid(Grid);
    clear D G I
    pause(1e-3)
    tic;
    [D,G,C,I,M] = build_ops(Grid);
    time(i) = toc;
    L = D*G;
    error_grad(i) = norm(dfdx(Grid.xf)-G*f(Grid.xc))/norm(dfdx(Grid.xf));
    error_lap(i) = norm(d2fdx2(Grid.xC)-D*G*f(Grid.xc))/
norm(d2fdx2(Grid.xc));
end
figure(4)
clf
subplot }12
loglog(Nx,error_grad,'ro','markerfacecolor','w'), hold on
loglog(Nx,error_lap,'bo','markerfacecolor',''w')
semilogy(Nx,Nx.^(-2)*1e2,'k--')
xlabel 'Nx', ylabel 'error'
xlim([Nx(1)-1e-3 Nx(end)+1e-3])
legend('gradient','Laplacian')
pbaspect([1 . 8 1])
subplot }12
loglog(Nx,time,'bo','markerfacecolor','w'), hold on
semilogy(Nx,min(time)*Nx/100, 'k-- ')
xlabel 'Nx', ylabel 'time [s]'
pbaspect([1 . 8 1])
```



The graph on the left shows the decline of the numerical error as a function of increasing grid refinement. The dashed line indicates the quadratic slope expected for that is expected for the central difference, which is second order accurate. Note, as the grid gets very fine ( $N>500,000$ ) the numerical rounding error takes over.

The graph on the right shows the time required to compute the discrete operators as the grid size increases with a dashed line indicating linear increase. The discrete opertors can be assemble very efficiently using the spdiags() function.

## Auxillary functions

```
function [] = set_defaults()
    set(0, ...
    'defaultaxesfontsize', 18, ...
    'defaultaxeslinewidth', 2.0, ...
    'defaultlinelinewidth', 2.0, ...
    'defaultpatchlinewidth', 2.0,...
    'DefaultLineMarkerSize', 12.0);
end
```

