Equation-Free function toolbox for Matlab/Octave

A. J. Roberts[*] et al.[†]

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Abstract

This 'equation-free toolbox' facilitates the computer-assisted analysis of complex, multiscale systems. Its aim is to enable microscopic simulators to perform system level tasks and analysis. The methodology bypasses the derivation of macroscopic evolution equations by using only short bursts of microscale simulations which are often the best available description of a system (Kevrekidis & Samaey 2009, Kevrekidis et al. 2004, 2003, e.g.). This suite of functions should empower users to start implementing such methods—but so far we have only just started.

Contents

[*] http://www.maths.adelaide.edu.au/anthony.roberts, http://orcid.org/0000-0001-8930-1552

[†] Be the first to appear here for your contribution.

3 Patch scheme for given microscale discrete space system

Section contents

The patch scheme applies to spatio-temporal systems where the spatial domain is larger than what can be computed in reasonable time. Then one may simulate only on small patches of the space-time domain, and produce correct macroscale predictions by craftily coupling the patches across unsimulated space (Hyman 2005, Samaey et al. 2005, 2006, Roberts & Kevrekidis 2007, Liu et al. 2015, e.g.).

The spatial discrete system is to be on a lattice such as obtained from finite difference approximation of a PDE. Usually continuous in time.

3.1 `patchSmooth1()`

Couples patches across space so a spatially discrete system can be integrated in time via the patch or gap-tooth scheme (Roberts & Kevrekidis 2007). Assumes that the sub-patch structure is *smooth* so that the patch centre-values are sensible macroscale variables, and patch edge values are determined by macroscale interpolation of the patch-centre values. Need to pass patch-design variables to this function, so use the global struct `patches`.

```
function dudt=patchSmooth1(t,u)
global patches
```

Input

- `u` is a vector of length `nSubP` · `nPatch` · `nVars` where there are `nVars` field values at each of the points in the `nSubP` × `nPatch` grid.
- `t` is the current time to be passed to the user's time derivative function.
- `patches` a struct set by `makePatches()` with the following information that is used here.
  - `.fun` is the name of the user's function `fun(t,u,x)` that computes the time derivatives on the patchy lattice. The array `u` has size `nSubP` × `nPatch` × `nVars`. Time derivatives must be computed into the same sized array, but the patch edge values will be overwritten by zeros.
  - `.x` is `nSubP` × `nPatch` array of the spatial locations x_{ij} of the microscale grid points in every patch. Currently it *must* be a regular lattice on both macro- and micro-scales.

Output

- `dudt` is `nSubP` · `nPatch` · `nVars` vector of time derivatives, but with zero on patch edges??

Reshape the fields `u` as a 2/3D-array, and sets the edge values from macroscale interpolation of centre-patch values. §3.3 describes function `patchEdgeInt1()`.

```
u=patchEdgeInt1(u);
```

Ask the user for the time derivatives computed in the array, overwrite its edge values with the dummy value of zero, then return to an integrator as column vector.

```
dudt=patches.fun(t,u,patches.x);
dudt([1 end],:,:)=0;
dudt=reshape(dudt,[],1);
```

Fin.

3.2 makePatches(): makes the spatial patches for the suite

Makes the struct `patches` for use by the patch/gap-tooth time derivative function `patchSmooth1()`.

```
function makePatches(fun,Xlim,BCs,nPatch,ordCC,ratio,nSubP)
global patches
```

Input

- `fun` is the name of the user function, `fun(t,u,x)`, that will compute time derivatives of quantities on the patches.
- `Xlim` give the macro-space domain of the computation: patches are spread evenly over the interior of the interval [`Xlim(1)`,`Xlim(2)`].
- `BCs` somehow will define the macroscale boundary conditions. Currently `BCs` is ignored and the system is assumed macro-periodic in the domain.
- `nPatch` is the number of evenly spaced patches.
- `ordCC` is the order of interpolation across empty space of the macroscale mid-patch values to the edge of the patches for inter-patch coupling: currently must be in $\{-1, 0, \dots, 8\}$.
- `ratio` (real) is the ratio of the half-width of a patch to the spacing of the patch mid-points: so `ratio` $= \frac{1}{2}$ means the patches abut; and `ratio` $= 1$ is overlapping patches as in holistic discretisation.
- `nSubP` is the number of microscale lattice points in each patch. Must be odd so that there is a central lattice point.

Output The *global* struct `patches` is created and set.

- `patches.fun` is the name of the user's function `fun(u,t,x)` that computes the time derivatives on the patchy lattice.
- `patches.ordCC` is the specified order of inter-patch coupling.
- `patches.alt` is true for interpolation using only odd neighbouring patches as for staggered grids, and false for the usual case of all neighbour coupling.
- `patches.Cwtsr` and `.Cwtsl` are the `ordCC`-vector of weights for the inter-patch interpolation onto the right and left edges (respectively) with patch:macroscale ratio as specified.
- `patches.x` is `nSubP` $\times$ `nPatch` array of the regular spatial locations x_{ij} of the microscale grid points in every patch.

First, store the pointer to the time derivative function in the struct.

```
patches.fun=fun;
```

Second, store the order of interpolation that is to provide the values for the inter-patch coupling conditions. Maybe allow `ordCC` of 0 and -1 to request spectral coupling??

```
if ~ismember(ordCC,[-1:8])
    error('makePatch: ordCC out of allowed range [-1:8]')
end
```

For odd `ordCC` do interpolation based upon odd neighbouring patches as is useful for staggered grids.

```
patches.alt=mod(ordCC,2);
ordCC=ordCC+patches.alt;
patches.ordCC=ordCC;
```

Check for staggered grid and periodic case.

```
  if patches.alt & (mod(nPatch,2)==1)
    error('Must have an even number of patches for a staggered grid'
```

```
  end
```

Might as well precompute the weightings for the interpolation of field values for coupling. (What about coupling via derivative values??)

```
if patches.alt  % eqn (7) in \cite{Cao2014a}
  patches.Cwtsr=[1
    ratio/2
    (-1+ratio^2)/8
    (-1+ratio^2)*ratio/48
    (9-10*ratio^2+ratio^4)/384
    (9-10*ratio^2+ratio^4)*ratio/3840
    (-225+259*ratio^2-35*ratio^4+ratio^6)/46080
    (-225+259*ratio^2-35*ratio^4+ratio^6)*ratio/645120 ];
else %
  patches.Cwtsr=[ratio
    ratio^2/2
    (-1+ratio^2)*ratio/6
    (-1+ratio^2)*ratio^2/24
    (4-5*ratio^2+ratio^4)*ratio/120
    (4-5*ratio^2+ratio^4)*ratio^2/720
    (-36+49*ratio^2-14*ratio^4+ratio^6)*ratio/5040
    (-36+49*ratio^2-14*ratio^4+ratio^6)*ratio^2/40320 ];
end
patches.Cwtsr=patches.Cwtsr(1:ordCC);
patches.Cwtsl=(-1).^((1:ordCC)'-patches.alt).*patches.Cwtsr;
```

Third, set the centre of the patches in a the macroscale grid of patches assuming periodic macroscale domain.

```
X=linspace(Xlim(1),Xlim(2),nPatch+1);
X=X(1:nPatch)+diff(X)/2;
DX=X(2)-X(1);
```

Construct the microscale in each patch, assuming Dirichlet patch edges, and a half-patch length of `ratio` · `DX`.

```
if mod(nSubP,2)==0, error('makePatches: nSubP must be odd'), end
```

```
i0=(nSubP+1)/2;
dx=ratio*DX/(i0-1);
patches.x=bsxfun(@plus,dx*(-i0+1:i0-1)',X); % micro-grid
```

Fin.

3.3 `patchEdgeInt1()`: sets edge values from macro-interpolation

Subsection contents

Couples patches across space by computing their edge values from macroscale interpolation. Consequently a spatially discrete system could be integrated in time via the patch or gap-tooth scheme (Roberts & Kevrekidis 2007). Assumes that the sub-patch structure is *smooth* so that the patch centre-values are sensible macroscale variables, and patch edge values are determined by macroscale interpolation of the patch-centre values. Pass patch-design variables via the global struct `patches`.

```
function u=patchEdgeInt1(u)
global patches
```

Input

- `u` is a vector of length `nSubP` · `nPatch` · `nVars` where there are `nVars` field values at each of the points in the `nSubP` × `nPatch` grid.
- `patches` a struct set by `makePatches()` with the following information.
  - `.fun` is the name of the user's function `fun(t,u,x)` that computes the time derivatives on the patchy lattice. The array `u` has size `nSubP` × `nPatch` × `nVars`. Time derivatives must be computed into the same sized array, but the patch edge values will be overwritten by zeros.

- `.x` is `nSubP` × `nPatch` array of the spatial locations x_{ij} of the microscale grid points in every patch. Currently it *must* be a regular lattice on both macro- and micro-scales.
- `.ordCC` is order of interpolation, currently in $\{0, 2, 4, 6, 8\}$.
- `.alt` in $\{0, 1\}$ is one for staggered grid (alternating) interpolation.
- `.Cwtsr` and `.Cwtsl`

Output

- `u` is `nSubP` × `nPatch` × `nVars` array of the fields with edge values set by interpolation.

Determine the sizes of things. Any error arising in the reshape indicates `u` has the wrong length.

```
[nM,nP]=size(patches.x);
nV=round(numel(u)/numel(patches.x));
u=reshape(u,nM,nP,nV);
```

With Dirichlet patches, the half-length of a patch is $h = dx(n_\mu - 1)/2$ (or -2 for specified flux), and the ratio needed for interpolation is then $r = h/\Delta X$. Compute lattice sizes from inside the patches as the edge values may be NaNs, etc.

```
dx=patches.x(3,1)-patches.x(2,1);
DX=patches.x(2,2)-patches.x(2,1);
r=dx*(nM-1)/2/DX;
```

For the moment?? assume the physical domain is macroscale periodic so that the coupling formulas are simplest. Should eventually cater for periodic, odd-mid-gap, even-mid-gap, even-mid-patch, dirichlet, neumann, ?? These index vectors point to patches and their two immediate neighbours.

```
j=1:nP; jp=mod(j,nP)+1; jm=mod(j-2,nP)+1;
```

The centre of each patch, assuming odd `nM`, is at

```
i0=round((nM+1)/2);
```

Lagrange interpolation gives patch-edge values So compute centred differences of the mid-patch values for the macro-interpolation, of all fields. Assumes the domain is macro-periodic.

```
if patches.ordCC>0 % then non-spectral interpolation
  dmu=nan(patches.ordCC,nP,nV);
  if patches.alt % use only odd numbered neighbours
    dmu(1,:,:)=(u(i0,jp,:)+u(i0,jm,:))/2; % \mu
    dmu(2,:,:)= u(i0,jp,:)-u(i0,jm,:); % \delta
    jp=jp(jp); jm=jm(jm); % increase shifts to \pm2
  else % standard
    dmu(1,:,:)=(u(i0,jp,:)-u(i0,jm,:))/2; % \mu\delta
    dmu(2,:,:)=(u(i0,jp,:)-2*u(i0,j,:)+u(i0,jm,:)); % \delta^2
  end% if odd/even
```

Recursively take δ^2 of these to form higher order centred differences (could unroll a little to cater for two in parallel).

```
  for k=3:patches.ordCC
    dmu(k,:,:)=dmu(k-2,jp,:)-2*dmu(k-2,j,:)+dmu(k-2,jm,:);
  end
```

Interpolate macro-values to be Dirichlet edge values for each patch (Roberts & Kevrekidis 2007), using weights computed in `makePatches()` . Here interpolate to specified order.

```
u(nM,j,:)=u(i0,j,:)*(1-patches.alt) ...
    +sum(bsxfun(@times,patches.Cwtsr,dmu));
u( 1,j,:)=u(i0,j,:)*(1-patches.alt) ...
    +sum(bsxfun(@times,patches.Cwtsl,dmu));
```

Case of spectral interpolation Assumes the domain is macro-periodic. As the macroscale fields are N-periodic, the macroscale Fourier transform writes the centre-patch values as $U_j = \sum_k C_k e^{ik2\pi j/N}$. Then the edge-patch values $U_{j\pm r} = \sum_k C_k e^{ik2\pi/N(j\pm r)} = \sum_k C'_k e^{ik2\pi j/N}$ where $C'_k = C_k e^{ikr2\pi/N}$. For nP patches we resolve 'wavenumbers' $|k| < \texttt{nP}/2$, so set row vector ks $= k2\pi/N$ for 'wavenumbers' $k = (0, 1, \ldots, k_{\max}, -k_{\max}, \ldots, -1)$.

```
else% spectral interpolation
```

Deal with staggered grid by doubling the number of fields and halving the number of patches (makePatches tests there are an even number of patches). Then the patch-ratio is effectively halved. The patch edges are near the middle of the gaps and swapped.

```
    if patches.alt % transform by doubling the number of fields
        v=nan(size(u)); % currently to restore the shape of u
        u=cat(3,u(:,1:2:nP,:),u(:,2:2:nP,:));
        altShift=reshape(0.5*[ones(nV,1);-ones(nV,1)],1,1,[]);
        iV=[nV+1:2*nV 1:nV]; % scatter interpolation to alternate fi
        r=r/2; % ratio effectively halved
        nP=nP/2; % halve the number of patches
        nV=nV*2; % double the number of fields
    else % the values for standard spectral
        altShift=0;
        iV=1:nV;
    end
```

Now set wavenumbers.

```
    kMax=floor((nP-1)/2);
    ks=2*pi/nP*(mod((0:nP-1)+kMax,nP)-kMax);
```

Test for reality of the field values, and define a function accordingly.

```
if imag(u(i0,:,:))==0, uclean=@(u) real(u);
    else                  uclean=@(u) u;
    end
```

Compute the Fourier transform of the patch centre-values for all the fields. If there are an even number of points, then zero the zig-zag mode in the FT and add it in later as cosine.

```
    Ck=fft(u(i0,:,:));
    if mod(nP,2)==0, Czz=Ck(1,nP/2+1,:)/nP; Ck(1,nP/2+1,:)=0; end
```

The inverse Fourier transform gives the edge values via a shift a fraction r to the next macroscale grid point. Enforce reality when appropriate.

```
    u(nM,:,iV)=uclean(ifft(bsxfun(@times,Ck ...
        ,exp(1i*bsxfun(@times,ks,altShift+r)))));
    u( 1,:,iV)=uclean(ifft(bsxfun(@times,Ck ...
        ,exp(1i*bsxfun(@times,ks,altShift-r)))));
```

For an even number of patches, add in the cosine mode.

```
    if mod(nP,2)==0
        cosr=cos(pi*(altShift+r+(0:nP-1)));
        u(nM,:,iV)=u(nM,:,iV)+uclean(bsxfun(@times,Czz,cosr));
        cosr=cos(pi*(altShift-r+(0:nP-1)));
        u( 1,:,iV)=u( 1,:,iV)+uclean(bsxfun(@times,Czz,cosr));
    end
```

Restore staggered grid when appropriate. Is there a better way to do this??

```
if patches.alt
    nV=nV/2;  nP=2*nP;
    v(:,1:2:nP,:)=u(:,:,1:nV);
    v(:,2:2:nP,:)=u(:,:,nV+1:2*nV);
    u=v;
end
end% if spectral
```

Fin, returning the 2/3D array of field values.

3.3.1 patchEdgeInt1test: test spectral interpolation

A script to test the spectral interpolation of function patchEdgeInt1() Establish global data struct for the range of various cases.

```
clear all
global patches
nSubP=3
i0=(nSubP+1)/2; % centre-patch index
```

Test standard spectral interpolation Test over various numbers of patches, random domain lengths and random ratios.

```
for nPatch=5:10
nPatch=nPatch
Len=10*rand
ratio=0.5*rand
makePatches(@sin,[0,Len],nan,nPatch,0,ratio,nSubP);
kMax=floor((nPatch-1)/2);
```

Test single field Set a profile, and evaluate the interpolation.

```
for k=-kMax:kMax
  u0=exp(1i*k*patches.x*2*pi/Len);
  ui=patchEdgeInt1(u0(:));
  normError=norm(ui-u0);
  if abs(normError)>5e-14
    normError=normError
    error(['failed single var interpolation k=' num2str(k)])
  end
end
```

Test multiple fields Set a profile, and evaluate the interpolation. For the case of the highest wavenumber, squash the error when the centre-patch values are all zero.

```
for k=1:nPatch/2
  u0=sin(k*patches.x*2*pi/Len);
  v0=cos(k*patches.x*2*pi/Len);
  uvi=patchEdgeInt1([u0(:);v0(:)]);
```

```
  normuError=norm(uvi(:,:,1)-u0)*norm(u0(i0,:));
  normvError=norm(uvi(:,:,2)-v0)*norm(v0(i0,:));
  if abs(normuError)+abs(normvError)>2e-13
    normuError=normuError, normvError=normvError
    error(['failed double field interpolation k=' num2str(k)])
  end
end
```

End the for-loop over various geometries.

```
end
```

Now test spectral interpolation on staggered grid Must have even number of patches for a staggered grid.

```
for nPatch=6:2:20
nPatch=nPatch
ratio=0.5*rand
nSubP=3; % of form 4*N-1
Len=10*rand
makePatches(@simpleWavepde,[0,Len],nan,nPatch,-1,ratio,nSubP);
kMax=floor((nPatch/2-1)/2)
```

Identify which microscale grid points are h or u values.

```
uPts=mod( bsxfun(@plus,(1:nSubP)',(1:nPatch)) ,2);
hPts=find(1-uPts);
uPts=find(uPts);
```

Set a profile for various wavenumbers. The capital letter `U` denotes an array of values merged from both u and h fields on the staggered grids.

```
fprintf('Single field-pair test.\n')
for k=-kMax:kMax
  U0=nan(nSubP,nPatch);
  U0(hPts)=rand*exp(+1i*k*patches.x(hPts)*2*pi/Len);
  U0(uPts)=rand*exp(-1i*k*patches.x(uPts)*2*pi/Len);
  Ui=patchEdgeInt1(U0(:));
```

```
  normError=norm(Ui-U0);
  if abs(normError)>5e-14
    normError=normError
    error(['failed single sys interpolation k=' num2str(k)])
  end
end
```

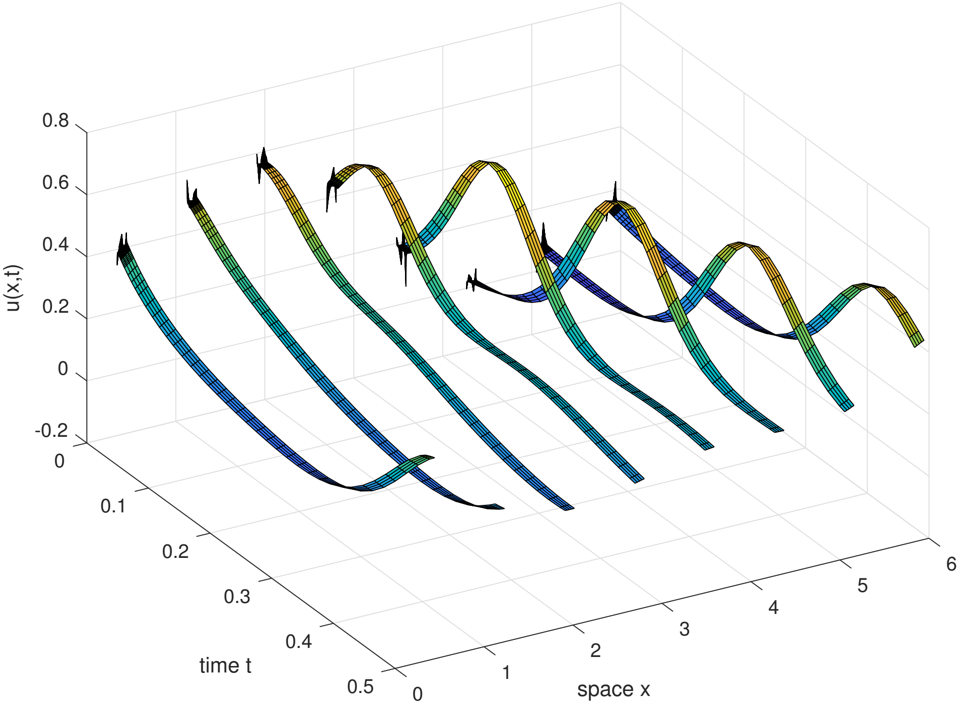
Test multiple fields Set a profile, and evaluate the interpolation. For the case of the highest wavenumber zig-zag, squash the error when the alternate centre-patch values are all zero. First shift the x-coordinates so that the zig-zag mode is centred on a patch.

```
fprintf('Two field-pairs test.\n')
x0=patches.x((nSubP+1)/2,1);
patches.x=patches.x-x0;
for k=1:nPatch/4
  U0=nan(nSubP,nPatch); V0=U0;
  U0(hPts)=rand*sin(k*patches.x(hPts)*2*pi/Len);
  U0(uPts)=rand*sin(k*patches.x(uPts)*2*pi/Len);
  V0(hPts)=rand*cos(k*patches.x(hPts)*2*pi/Len);
  V0(uPts)=rand*cos(k*patches.x(uPts)*2*pi/Len);
  UVi=patchEdgeInt1([U0(:);V0(:)]);
  normuError=norm(UVi(:,1:2:nPatch,1)-U0(:,1:2:nPatch))*norm(U0(i0,2
      +norm(UVi(:,2:2:nPatch,1)-U0(:,2:2:nPatch))*norm(U0(i0,1:2:nPa
  normuError=norm(UVi(:,1:2:nPatch,2)-V0(:,1:2:nPatch))*norm(V0(i0,2
      +norm(UVi(:,2:2:nPatch,2)-V0(:,2:2:nPatch))*norm(V0(i0,1:2:nPa
  if abs(normuError)+abs(normvError)>2e-13
    normuError=normuError, normvError=normvError
    error(['failed double field interpolation k=' num2str(k)])
  end
end
```

End for-loop over patches

```
end
```

Figure 7: field $u(x,t)$ tests the patch scheme function applied to Burgers' PDE.



Finish If no error messages, then all OK.

```
fprintf('\nIf you read this, then all tests were passed\n')
```

3.4 `BurgersExample`: simulate Burgers' PDE on patches

Figure 7 shows an example simulation in time generated by the patch scheme function applied to Burgers' PDE. The inter-patch coupling is realised by fourth-order interpolation to the patch edges of the mid-patch values.

```
function BurgersExample
```

Establish global data struct for Burgers' PDE solved on 2π-periodic domain, with eight patches, each patch of half-size ratio 0.2, with seven points within each patch, and say fourth order/spectral interpolation provides values for the inter-patch coupling conditions.

```
global patches
nPatch=8
ratio=0.2
nSubP=7
Len=2*pi;
interpOrd=0
makePatches(@burgerspde,[0,Len],nan,nPatch,interpOrd,ratio,nSubP);
```

Set an initial condition, and check evaluation of the time derivative.

```
u0=0.3*(1+sin(patches.x))+0.05*randn(size(patches.x));
dudt=patchSmooth1(0,u0(:));
```

Conventional integration in time Integrate in time using standard Matlab/Octave functions.

```
ts=linspace(0,0.5,60);
if exist('OCTAVE_VERSION', 'builtin') % Octave version
   ucts=lsode(@(u,t) patchSmooth1(t,u),u0(:),ts);
else % Matlab version
   [ts,ucts]=ode15s(@patchSmooth1,ts([1 end]),u0(:));
end
```

Plot the simulation, but here use only the microscale values interior to the patches. Use `nan` in the x-edges to leave gaps.

```
figure(1),clf
xs=patches.x; xs([1 end],:)=nan;
surf(ts,xs(:),ucts')
title('Use standard integrators for stiff systems')
xlabel('time t'), ylabel('space x'), zlabel('interior field u(x,t)')
view(60,40)
%print('-depsc2','ps1BurgersCtsU')
```

Alternatively, plot all the patch values via interpolation. Usually want to seperate the patches by gaps using `nan`.

```
figure(2),clf()
u=patchEdgeInt1(ucts');
u=[u; nan(1,size(u,2),size(u,3))];
xs=[patches.x; nan(1,size(patches.x,2))];
surf(ts,xs(:),reshape(u,[],length(ts)))
title('Use standard integrators for stiff systems')
xlabel('time t'), ylabel('space x'), zlabel('field u(x,t)')
view(60,40)
```

Exit now until we get the new projective integration working.

```
return
```

Use projective integration Now wrap around the patch time derivative function, `patchSmooth1`, the projective integration function for patch simulations as illustrated by Figure 8.

Mark that edge of patches are not to be used in the projective extrapolation by setting initial values to NaN.

```
u0([1 end],:)=nan;
```

Set the desired macro- and micro-scale time-steps over the time domain.

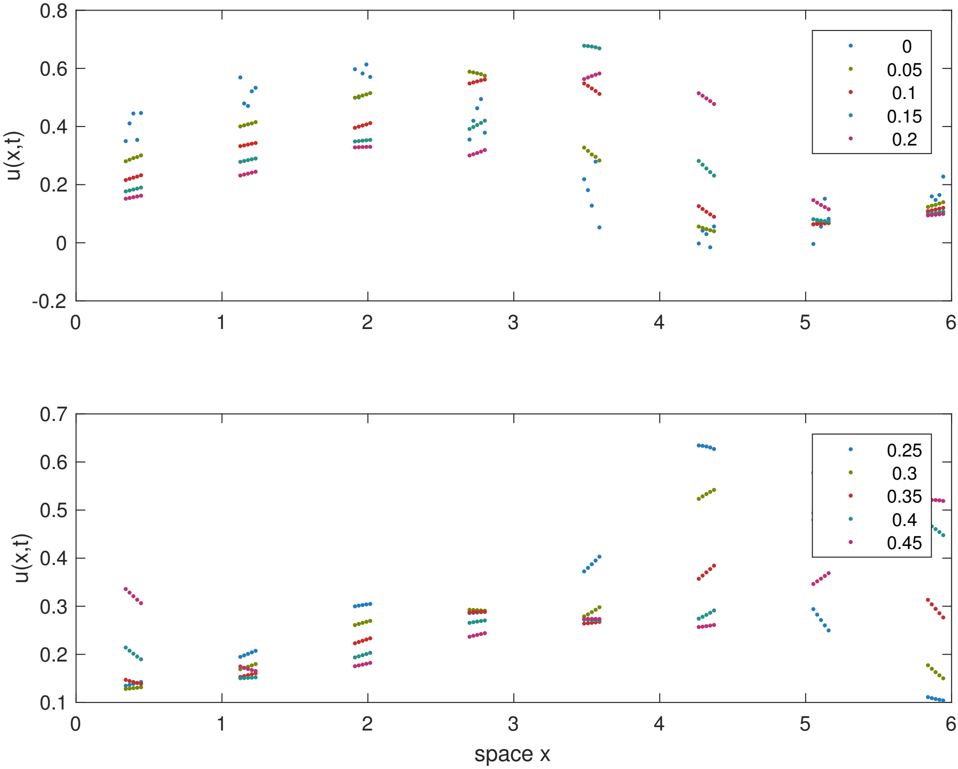
```
ts=linspace(0,0.45,10)
dt=0.4*(ratio*Len/nPatch/(nSubP/2-1))^2;
```

Projectively integrate in time with: DMD projection of rank `nPatch` $+ 1$; guessed microscale time-step `dt`; and guessed numbers of transient and slow steps.

```
addpath('../ProjInt')
[us,uss,tss]=projInt1(@patchSmooth1,u0(:),ts ...
    ,nPatch+1,dt,[20 nPatch*2]);
```

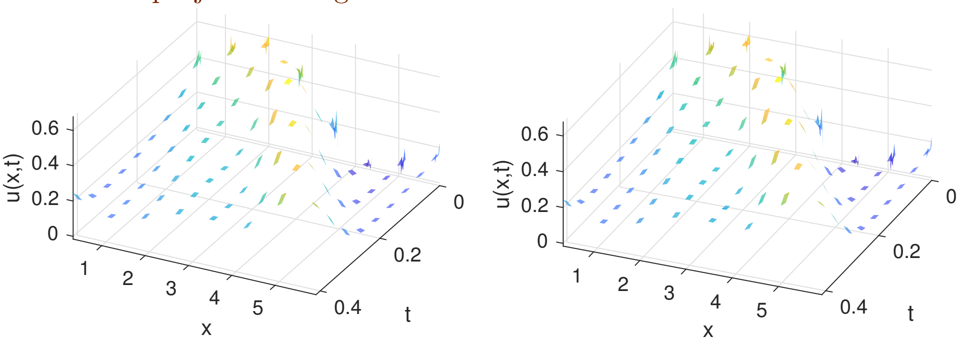
Plot the macroscale predictions to draw Figure 8, in groups of five in a plot.

Figure 8: field $u(x,t)$ tests basic projective integration of the patch scheme function applied to Burgers' PDE.




```
figure(2),clf
k=length(ts); ls=nan(5,ceil(k/5)); ls(1:k)=1:k;
for k=1:size(ls,2)
  subplot(size(ls,2),1,k)
  plot(xs(:),us(:,ls(:,k)),'.')
  ylabel('u(x,t)')
  legend(num2str(ts(ls(:,k))'))
end
xlabel('space x')
%print('-depsc2','ps1BurgersU')
```

Figure 9: stereo pair of the field $u(x,t)$ during each of the microscale bursts used in the projective integration.



Also plot a surface of the microscale bursts as shown in Figure 9.

```
tss(end)=nan; %omit end time-point
figure(3),clf
for k=1:2, subplot(2,2,k)
  surf(tss,xs(:),uss,'EdgeColor','none')
  ylabel('x'),xlabel('t'),zlabel('u(x,t)')
  axis tight, view(121-4*k,45)
end
%print('-depsc2','ps1BurgersMicro')
```

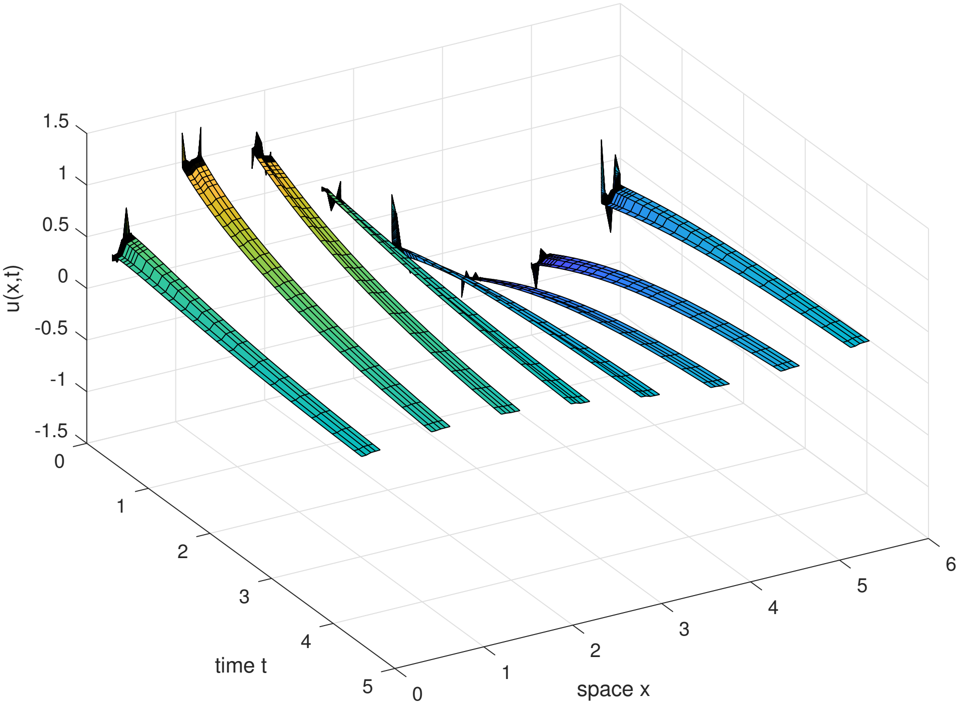
End the main function

```
end
```

This function codes the lattice equation inside the patches.

```
function ut=burgerspde(t,u,x)
dx=x(2)-x(1);
ut=nan(size(u));
i=2:size(u,1)-1;
ut(i,:)=diff(u,2)/dx^2 ...
   -30*u(i,:).*(u(i+1,:)-u(i-1,:))/(2*dx);
end
```

Figure 10: field $u(x,t)$ tests the patch scheme function applied to heterogeneous diffusion.



Fin.

3.5 `HomogenisationExample`: simulate heterogeneous diffusion in 1D on patches

Figure 10 shows an example simulation in time generated by the patch scheme function applied to heterogeneous diffusion. The inter-patch coupling is realised by fourth-order interpolation to the patch edges of the mid-patch values.

```
function HomogenisationExample
```

Consider a lattice of values $u_i(t)$, with lattice spacing dx, and governed by the heterogeneous diffusion

$$\dot{u}_i = [c_{i-1/2}(u_{i-1} - u_i) + c_{i+1/2}(u_{i+1} - u_i)]/dx^2.$$

The macroscale, homogenised, effective diffusion should be the harmonic mean of these coefficients. Set the desired microscale periodicity, and microscale diffusion coefficients (with subscripts shifted by a half).

```
mPeriod=3
cDiff=2*rand(mPeriod,1)
cHomo=1/mean(1./cDiff)
```

Establish global data struct for heterogeneous diffusion solved on 2π-periodic domain, with eight patches, each patch of half-size 0.1, and the number of points in a patch being one more than an even multiple of the microscale periodicity (which Bunder et al. (2017) showed is accurate). Fourth order interpolation provides values for the inter-patch coupling conditions.

```
global patches
nPatch=8
ratio=0.2
nSubP=2*mPeriod+1
Len=2*pi;
makePatches(@heteroDiff,[0,Len],nan,nPatch,4,ratio,nSubP);
```

Can add to the global data struct `patches` for use by the time derivative function (for example): here include the diffusivity coefficients, repeated to fill up a patch.

```
patches.c=repmat(cDiff,(nSubP-1)/mPeriod,1);
```

Set an initial condition, and test evaluation of the time derivative.

```
u0=sin(patches.x)+0.2*randn(size(patches.x));
dudt=patchSmooth1(0,u0(:));
```

Conventional integration in time Integrate in time using standard Matlab/Octave functions.

```
ts=linspace(0,2/cHomo,60);
if exist('OCTAVE_VERSION', 'builtin') % Octave version
   ucts=lsode(@(u,t) patchSmooth1(t,u),u0(:),ts);
else % Matlab version
   [ts,ucts]=ode15s(@patchSmooth1,ts([1 end]),u0(:));
end
```

Plot the simulation.

```
figure(1),clf
xs=patches.x; xs([1 end],:)=nan;
surf(ts,xs(:),ucts')
xlabel('time t'),ylabel('space x'),zlabel('u(x,t)')
view(60,40)
%print('-depsc2','ps1HomogenisationCtsU')
```

Use projective integration Now wrap around the patch time derivative function, `patchSmooth1`, the projective integration function for patch simulations as illustrated by Figure 11.

Mark that edge of patches are not to be used in the projective extrapolation by setting initial values to NaN.

```
u0([1 end],:)=nan;
```

Set the desired macro- and micro-scale time-steps over the time domain.

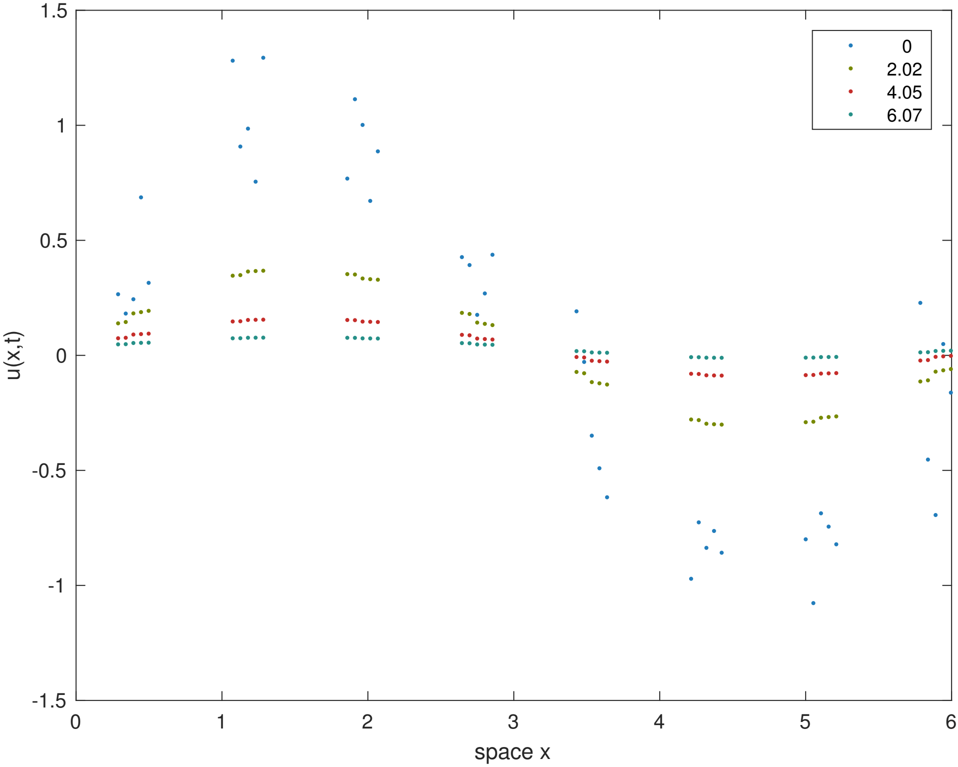
```
ts=linspace(0,3/cHomo,4)
dt=0.4*(ratio*Len/nPatch/(nSubP/2-1))^2/max(cDiff);
```

Projectively integrate in time with: DMD projection of rank `nPatch` $+ 1$; guessed microscale time-step `dt`; and guessed numbers of transient and slow steps.

```
addpath('../ProjInt')
[us,uss,tss]=projInt1(@patchSmooth1,u0(:),ts ...
    ,nPatch+1,dt,[20 nPatch*2]);
```

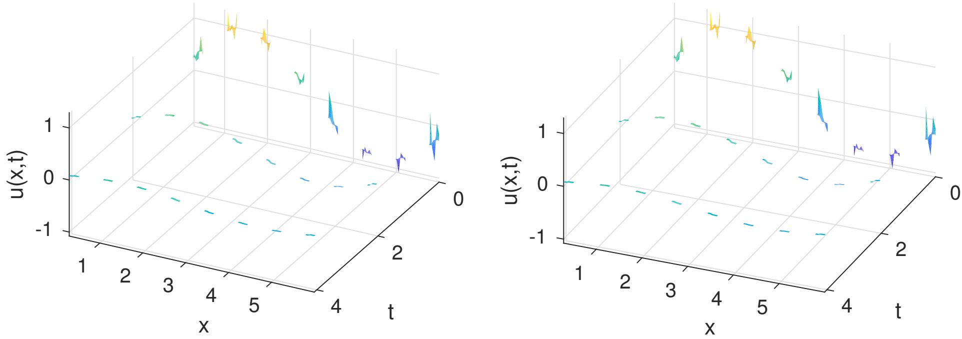
Plot the macroscale predictions to draw Figure 11, in groups of five in a plot.

Figure 11: field $u(x,t)$ tests basic projective integration of the patch scheme function applied to heterogeneous diffusion.




```
figure(2),clf
k=length(ts); ls=nan(5,ceil(k/5)); ls(1:k)=1:k;
for k=1:size(ls,2)
  subplot(size(ls,2),1,k)
  plot(xs(:),us(:,ls(~isnan(ls(:,k)),k)),'.')
  ylabel('u(x,t)')
  legend(num2str(ts(ls(~isnan(ls(:,k)),k))',3))
end
xlabel('space x')
%print('-depsc2','ps1HomogenisationU')
```

Figure 12: stereo pair of the field $u(x,t)$ during each of the microscale bursts used in the projective integration.



Also plot a surface of the microscale bursts as shown in Figure 12.

```
tss(end)=nan; %omit end time-point
figure(3),clf
for k=1:2, subplot(2,2,k)
  surf(tss,xs(:),uss,'EdgeColor','none')
  ylabel('x'),xlabel('t'),zlabel('u(x,t)')
  axis tight, view(121-4*k,45)
end
%print('-depsc2','ps1HomogenisationMicro')
```

End the main function

```
end
```

This function codes the lattice heterogeneous diffusion inside the patches.

```
function ut=heteroDiff(t,u,x)
global patches
dx=patches.x(2)-patches.x(1);
ut=nan(size(u));
i=2:size(u,1)-1;
ut(i,:)=diff(bsxfun(@times,patches.c,diff(u)))/dx^2 ;
end
```

Fin.

3.6 `waterWaveExample`: simulate a water wave PDE on patches

Subsection contents

Figure 13 shows an example simulation in time generated by the patch scheme function applied to a simple wave PDE. The inter-patch coupling is realised by third-order interpolation to the patch edges of the mid-patch values.

This section describes the nonlinear microscale simulator of the nonlinear shallow water wave PDE derived from the Smagorinski model of turbulent flow (Cao & Roberts 2012, 2016*a*). Often, wave-like systems are written in terms of two conjugate variables, for example, position and momentum density, electric and magnetic fields, and water depth $h(x,t)$ and mean lateral velocity $u(x,t)$ as herein. The approach applies to any wave-like system in the form

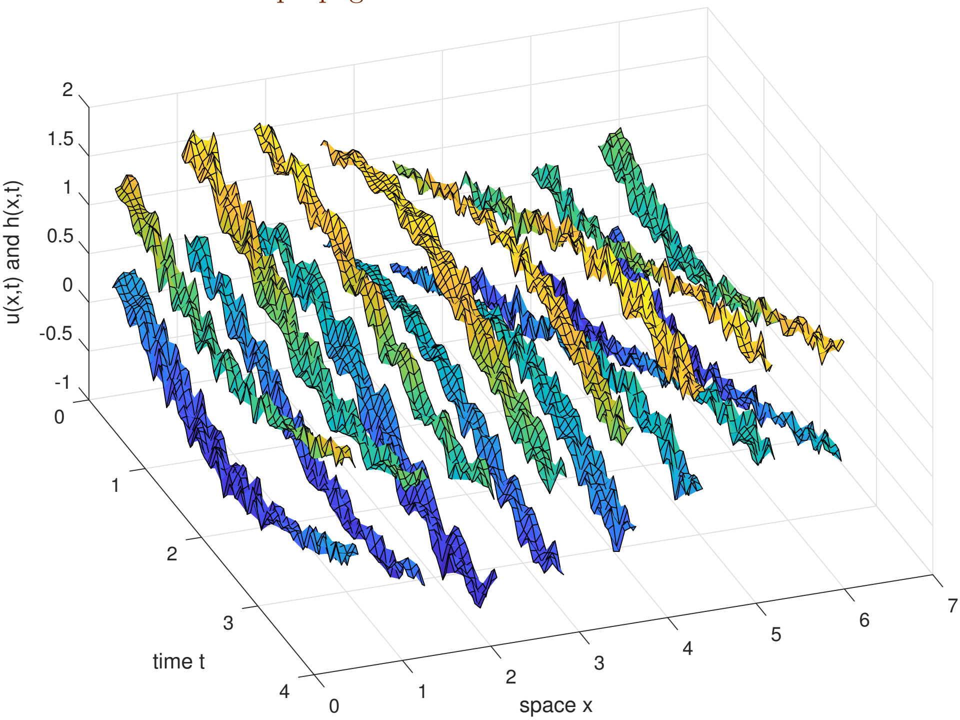
$$\frac{\partial h}{\partial t}=-c_1\frac{\partial u}{\partial x}+f_1[h,u] \quad\text{and}\quad \frac{\partial u}{\partial t}=-c_2\frac{\partial h}{\partial x}+f_2[h,u], \tag{1}$$

where the brackets indicate that the nonlinear functions f_ℓ may involve various spatial derivatives of the fields $h(x,t)$ and $u(x,t)$. Specifically, this section invokes a nonlinear Smagorinski model of turbulent shallow water (Cao & Roberts 2012, 2016*a*, e.g.) along an inclined flat bed: let x measure position along the bed and in terms of fluid depth $h(x,t)$ and depth-averaged lateral velocity $u(x,t)$ the model PDEs are

$$\frac{\partial h}{\partial t}=-\frac{\partial(hu)}{\partial x}\,, \tag{2a}$$

$$\frac{\partial u}{\partial t}=0.985\left(\tan\theta-\frac{\partial h}{\partial x}\right)-0.003\frac{u|u|}{h}-1.045u\frac{\partial u}{\partial x}+0.26h|u|\frac{\partial^2 u}{\partial x^2}\,, \tag{2b}$$

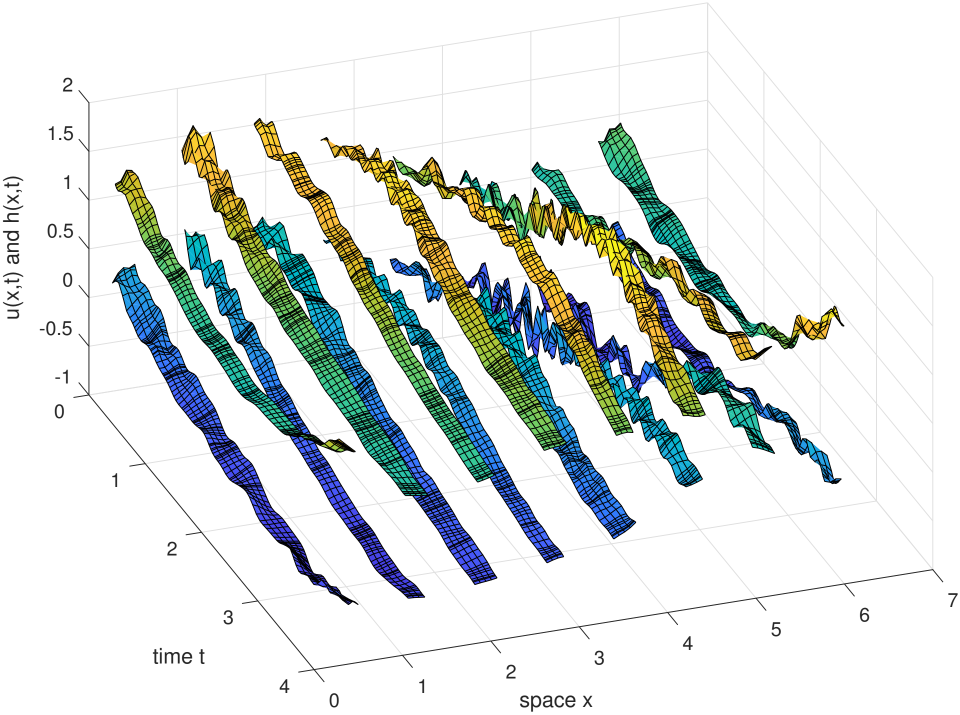
Figure 13: water depth $h(x,t)$ (above) and velocity field $u(x,t)$ (below) of the gap-tooth scheme function applied to simple wave PDE. A random component to the initial condition has long lasting effects on the simulation—but the macroscale wave still propagates.



where $\tan\theta$ is the slope of the bed. Equation (2a) represents conservation of the fluid. The momentum PDE (2b) represents the effects of turbulent bed drag $u|u|/h$, self-advection $u\partial u/\partial x$, nonlinear turbulent dispersion $h|u|\partial^2 u/\partial x^2$, and gravitational hydrostatic forcing $\tan\theta - \partial h/\partial x$. Figure 14 shows one simulation of this system—for the same initial condition as Figure 13.

For such wave systems, let's try a staggered microscale grid and staggered macroscale patches as introduced in Figures 3 and 4, respectively, by Cao & Roberts (2016*b*).

Figure 14: water depth $h(x,t)$ (above) and velocity field $u(x,t)$ (below) of the gap-tooth scheme the shallow water wave PDEs (2). A random component decays where the speed is non-zero.




```
function waterWaveExample
```

Establish global data struct for the PDEs (2) solved on 2π-periodic domain, with eight patches, each patch of half-size 0.2, with eleven points within each patch, and third-order interpolation provides values for the inter-patch coupling conditions (higher order interpolation is smoother for these smooth initial conditions).

```
global patches
nPatch=8
ratio=0.2
```

```
nSubP=11 % of form 4*?-1
Len=2*pi;
makePatches(@simpleWavepde,[0,Len],nan,nPatch,3,ratio,nSubP);
```

Identify which microscale grid points are h or u values. Also store them in the struct `patches` for use by the time derivative function.

```
uPts=mod( bsxfun(@plus,(1:nSubP)',(1:nPatch)) ,2);
hPts=find(1-uPts);
uPts=find(uPts);
patches.hPts=hPts; patches.uPts=uPts;
```

Set an initial condition of a progressive wave, and check evaluation of the time derivative. The capital letter `U` denotes an array of values merged from both u and h fields on the staggered grids.

```
U0=nan(nSubP,nPatch);
U0(hPts)=1+0.5*sin(patches.x(hPts));
U0(uPts)=0+0.5*sin(patches.x(uPts));
U0=U0+0.05*randn(nSubP,nPatch);
dUdt0=patchSmooth1(0,U0(:));% check
%dUdt0=reshape(dUdt0,nSubP,nPatch)
```

Conventional integration in time Integrate in time using standard Matlab/Octave functions the two cases of the simple wave equations and the water wave equations.

```
for k=1:2
```

When using `ode15s` we subsample the results because the sub-grid scale waves do not dissipate and so the integrator takes very small time steps for all time.

```
ts=linspace(0,4,41);
if exist('OCTAVE_VERSION', 'builtin') % Octave version
   Ucts=lsode(@(u,t) patchSmooth1(t,u),U0(:),ts);
else % Matlab version
   [ts,Ucts]=ode15s(@patchSmooth1,ts([1 end]),U0(:));
```

```
    ts=ts(1:5:end);
    Ucts=Ucts(1:5:end,:);
end
```

Plot the simulation.

```
figure(k),clf
xs=patches.x; xs([1 end],:)=nan;
surf(ts,xs(patches.hPts),Ucts(:,patches.hPts)'),hold on
surf(ts,xs(patches.uPts),Ucts(:,patches.uPts)'),hold off
xlabel('time t'),ylabel('space x'),zlabel('u(x,t) and h(x,t)')
view(70,45)
```

Print the graph.

```
if k==1, print('-depsc2','ps1WaveCtsUH')
else print('-depsc2','ps1WaterWaveCtsUH')
end
```

Now, change to the Smagorinski turbulence model (2) of shallow water flow, keeping other parameters and the initial condition the same. And end the loop to redo the simulation.

```
patches.fun=@waterWavepde;
dUdt0=patchSmooth1(0,U0(:));%check
end
```

Use projective integration As yet a simple implementation appears to fail, so it needs more exploration and thought.

End the main function

```
end
```

3.6.1 Simple wave PDE

This function codes the staggered lattice equation inside the patches for the simple wave PDE system $h_t = -u_x$ and $u_t = -h_x$. Here code for a staggered microscale grid of staggered macroscale patches: the array

$$U_{ij} = \begin{cases} u_{ij} & i+j \text{ even,} \\ h_{ij} & i+j \text{ odd.} \end{cases}$$

The output `Ut` contains the merged time derivatives of the two staggered fields. So set the micro-grid spacing and reserve space for time derivatives.

```
function Ut=simpleWavepde(t,U,x)
global patches
dx=x(2)-x(1);
Ut=nan(size(U));
ht=Ut;
```

Compute the PDE derivatives at points internal to the patches.

```
i=2:size(U,1)-1;
```

Here ‘wastefully’ compute time derivatives for both PDEs at all grid points—for ‘simplicity’—and then merges the staggered results. Since $\dot h_{ij} \approx -(u_{i+1,j} - u_{i-1,j})/(2 \cdot dx) = -(U_{i+1,j} - U_{i-1,j})/(2 \cdot dx)$ as adding/subtracting one from the index of a h-value is the location of the neighbouring u-value on the staggered micro-grid.

```
ht(i,:)=-(U(i+1,:)-U(i-1,:))/(2*dx);
```

Since $\dot u_{ij} \approx -(h_{i+1,j} - h_{i-1,j})/(2 \cdot dx) = -(U_{i+1,j} - U_{i-1,j})/(2 \cdot dx)$ as adding/subtracting one from the index of a u-value is the location of the neighbouring h-value on the staggered micro-grid.

```
Ut(i,:)=-(U(i+1,:)-U(i-1,:))/(2*dx);
```

Then overwrite the unwanted $\dot u_{ij}$ with the corresponding wanted $\dot h_{ij}$.

```
Ut(patches.hPts)=ht(patches.hPts);
end
```

3.6.2 Water wave PDE

This function codes the staggered lattice equation inside the patches for the nonlinear wave-like PDE system (2). As before, set the micro-grid spacing, reserve space for time derivatives, and index the internal points of the micro-grid.

```
function Ut=waterWavepde(t,U,x)
global patches
dx=x(2)-x(1);
Ut=nan(size(U));
ht=Ut;
i=2:size(U,1)-1;
```

Need to estimate h at all the u-points, so into `V` use averages, and linear extrapolation to patch-edges.

```
ii=i(2:end-1);
V=Ut;
V(ii,:)=(U(ii+1,:)+U(ii-1,:))/2;
V(1:2,:)=2*U(2:3,:)-V(3:4,:);
V(end-1:end,:)=2*U(end-2:end-1,:)-V(end-3:end-2,:);
```

Then estimate $\partial hu/\partial x$ from u and the interpolated h at the neighbouring micro-grid points.

```
ht(i,:)=-(U(i+1,:).*V(i+1,:)-U(i-1,:).*V(i+1,:))/(2*dx);
```

Correspondingly estimate the terms in the momentum PDE: u-values in $\texttt{U}_i$ and $\texttt{V}_{i\pm1}$; and h-values in $\texttt{V}_i$ and $\texttt{U}_{i\pm1}$.

```
Ut(i,:)=-0.985*(U(i+1,:)-U(i-1,:))/(2*dx) ...
    -0.003*U(i,:).*abs(U(i,:)./V(i,:)) ...
    -1.045*U(i,:).*(V(i+1,:)-V(i-1,:))/(2*dx) ...
    +0.26*abs(V(i,:).*U(i,:)).*(V(i+1,:)-2*U(i,:)+V(i-1,:))/dx^2/2;
```

where the mysterious division by two in the 2nd derivative is due to using the averaged values of u in the estimate:

$$\begin{aligned} u_{xx} &\approx \frac{1}{4\delta^2}(u_{i-2} - 2u_i + u_{i+2}) \\ &= \frac{1}{4\delta^2}(u_{i-2} + u_i - 4u_i + u_i + u_{i+2}) \\ &= \frac{1}{2\delta^2}\left(\frac{u_{i-2} + u_i}{2} - 2u_i + \frac{u_i + u_{i+2}}{2}\right) \\ &= \frac{1}{2\delta^2}\left(\bar u_{i-1} - 2u_i + \bar u_{i+1}\right). \end{aligned}$$

Then overwrite the unwanted $\dot u_{ij}$ with the corresponding wanted $\dot h_{ij}$.

```
Ut(patches.hPts)=ht(patches.hPts);
end
```

Fin.

3.7 To do

- Testing is so far only qualitative. Need to be quantitative.
- Multiple space dimensions.
- Heterogeneous microscale via averaging regions.
- Parallel processing versions.
- ??
- Adapt to maps in micro-time?

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