Equation-free computational homogenisation with various boundaries and various patch spacing

A. J. Roberts*

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*School of Mathematical Sciences, University of Adelaide, South Australia. https://profajroberts.github.io, http://orcid.org/0000-0001-8930-1552

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Examples

1 `Eckhardt2210eg2`: example of a 1D heterogeneous diffusion by simulation on small patches

Plot an example simulation in time generated by the patch scheme applied to macroscale forced diffusion through a medium with microscale heterogeneity in space. This is more-or-less the second example of Eckhardt and Verfürth (2022) [§6.2.1].

Suppose the spatial microscale lattice is at points x_i, with constant spacing dx. With dependent variables $u_i(t)$, simulate the microscale lattice forced diffusion system

$$\frac{\partial u_i}{\partial t} = \frac{1}{dx^2}\delta[a_{i-1/2}\delta u_i] + f_i(t), \tag{1}$$

in terms of the centred difference operator δ. The system has a microscale heterogeneity via the coefficients $a_{i+1/2}$ which has some given known periodicity ϵ.

Here use period $\epsilon = 1/130$ (so that computation completes in seconds). The patch scheme computes only on a fraction of the spatial domain, see Figure 1. Compute *errors* as the maximum difference (at time $t = 1$) between the patch scheme prediction and a full-domain simulation of the same underlying spatial discretisation (which here has space step 0.00128).

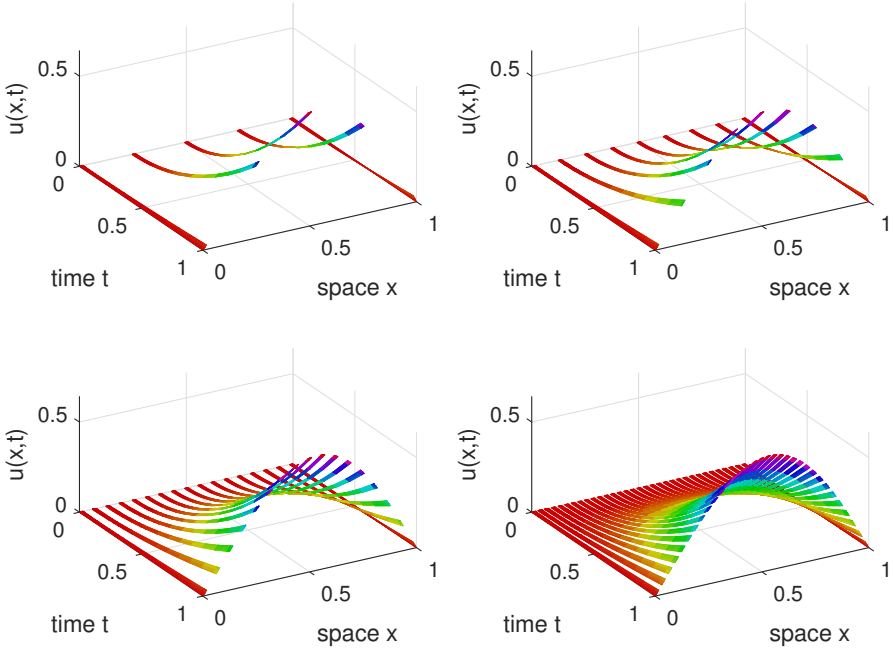
patch spacing H	0.25	0.12	0.06	0.03
exp-sine-forcing error	8E−3	2E−3	3E−4	2E−5
parabolic-forcing error	9E−9	4E−9	1E−9	0.06E−9

The smooth sine-forcing leads to errors that appear due to patch scheme and its interpolation. The parabolic-forcing errors appear to be due to the integration errors of `ode15s` and not at all due to the patch scheme. In comparison, Eckhardt and Verfürth (2022) reported much larger errors in the range 0.001–0.1 (Figure 3).

1.1 Simulate heterogeneous diffusion systems

First establish the microscale heterogeneity has micro-period `mPeriod` on the lattice, and coefficients to match Eckhardt2210.04536 §6.2.1. Set the phase of the heterogeneity so that each patch centre is a point of symmetry of the diffusivity. Then the heterogeneity is repeated to fill each patch.

Figure 1: diffusion field $u(x,t)$ of the patch scheme applied to the forced heterogeneous diffusive (1). Simulate for $5, 9, 17, 33$ patches and compare to the full-domain simulation (65 patches, not shown).




```
clear all
%global OurCf2eps, OurCf2eps=true %option to save plots
mPeriod = 6
y = linspace(0,1,mPeriod+1)';
a = 1./(2-cos(2*pi*y(1:mPeriod)))
global microTimePeriod; microTimePeriod=0;
```

Set the spatial period ϵ, via integer $1/\epsilon$, and other parameters.

```
maxLog2Nx = 6
nPeriodsPatch = 2 % any integer
rEpsilon = nPeriodsPatch*(2^maxLog2Nx+1) % up to 200 say
dx = 1/(mPeriod*rEpsilon+1)
nSubP = nPeriodsPatch*mPeriod+2
tol=1e-9;
```

Loop to explore errors on various sized patches.

```
Us=[]; DXs=[]; % for storing results to compare
iPP=0; I=nan;
for log2Nx = 2:maxLog2Nx
    nP = 2^log2Nx+1
```

Determine indices of patches that are common in various resolutions

```
    if isnan(I), I=1:nP; else I=2*I-1; end
```

Establish the global data struct `patches` for the microscale heterogeneous lattice diffusion system (1) solved on domain $[0, 1]$, with `nP` patches, and say fourth order interpolation to provide the edge-values. Setting `patches.EdgyInt` true means the edge-values come from interpolating the opposite next-to-edge values of the patches (not the mid-patch values).

```
    global patches
    ordCC = 4
    configPatches1(@heteroDiffF,[0 1],'equispace',nP ...
        ,ordCC,dx,nSubP,'EdgyInt',true,'hetCoeffs',a);
    DX = mean(diff(squeeze(patches.x(1,1,1,:))))
    DXs=[DXs;DX];
```

Set the forcing coefficients, either the original parabolic, or exp-sinusoidal.

```
    if 0 % given forcing is exact
      patches.f1=2*( patches.x-patches.x.^2 );
      patches.f2=2*0.5+0*patches.x;
    else% simple exp.sine forcing
      patches.f1=sin(pi*patches.x).*exp(patches.x);
      patches.f2=pi/2*sin(pi*patches.x).*exp(patches.x);
    end%if
```

Simulate Set the initial conditions of a simulation to be zero. Integrate to time 1 using standard integrators.

```
    u0 = 0*patches.x;
    tic
    [ts,us] = ode15s(@patchSys1, [0 1], u0(:));
    cpuTime=toc
```

Plot space-time surface of the simulation We want to see the edge values of the patches, so adjoin a row of `nan`s in between patches. For the field values (which are rows in `us`) we need to reshape, permute, interpolate to get edge values, pad with `nan`s, and reshape again.

```
    xs = squeeze(patches.x);
    us = patchEdgeInt1( permute( reshape(us ...
        ,length(ts),nSubP,1,nP) ,[2 1 3 4]) );
    us = squeeze(us);
    xs(end+1,:) = nan;  us(end+1,:,:) = nan;
    uss=reshape(permute(us,[1 3 2]),[],length(ts));
```

Plot a space-time surface of field values over the macroscale duration of the simulation.

```
    iPP=iPP+1;
    if iPP<=4 % only draw four subplots
      figure(1), if iPP==1, clf(), end
      subplot(2,2,iPP)
      mesh(ts,xs(:),uss)
      if iPP==1, uMax=ceil(max(uss(:))*100)/100, end
      view(60,40), colormap(0.8*hsv), zlim([0 uMax])
      xlabel('time t'), ylabel('space x'), zlabel('u(x,t)')
      drawnow
    end%if
```

At the end of the `log2Nx`-loop, store field at the end-time from centre region of each patch for comparison.

```
    i=nPeriodsPatch/2*mPeriod+1+(-mPeriod/2+1:mPeriod/2);
    Us(:,:,iPP)=squeeze(us(i,end,I));
    Xs=squeeze(patches.x(i,1,1,I));
    if iPP>1
       assert(norm(Xs-Xsp)<tol,'sampling error in space')
       end
    Xsp=Xs;
end%for log2Nx
ifOurCf2eps(mfilename) %optionally save plot
```

Assess errors by comparing to the full-domain solution

```
DXs=DXs
Uerr=squeeze(max(max(abs(Us-Us(:,:,end)))))
figure(2),clf,
loglog(DXs,Uerr,'o:')
xlabel('H'),ylabel('error')
ifOurCf2eps([mfilename 'Errs']) %optionally save plot
```

1.2 `heteroDiffF()`: forced heterogeneous diffusion

This function codes the lattice heterogeneous diffusion inside the patches with forcing and with microscale boundary conditions on the macroscale boundaries. Computes the time derivative at each point in the interior of a patch, output in `ut`. The column vector of diffusivities a_i has been stored in struct `patches.cs`, as has the array of forcing coefficients.

```
function ut = heteroDiffF(t,u,patches)
```

Cater for the two cases: one of a non-autonomous forcing oscillating in time when `microTimePeriod` > 0, or otherwise the case of an autonomous diffusion constant in time.

```
  global microTimePeriod
  if microTimePeriod>0 % optional time fluctuations
     at = cos(2*pi*t/microTimePeriod)/30;
  else at=0; end
```

Two basic parameters, and initialise result array to NaNs.

```
  dx = diff(patches.x(2:3));   % space step
  i = 2:size(u,1)-1;   % interior points in a patch
  ut = nan+u;          % preallocate output array
```

The macroscale Dirichlet boundary conditions are zero at the extreme edges of the two extreme patches.

```
  u( 1 ,:,:, 1 )=0; % left-edge of leftmost is zero
  u(end,:,:,end)=0; % right-edge of rightmost is zero
```

Code the microscale forced diffusion.

```
  ut(i,:,:,:) = diff((patches.cs(:,1,:)+at).*diff(u))/dx^2 ...
      +patches.f2(i,:,:,:)*t^2+patches.f1(i,:,:,:)*t;
end% function
```

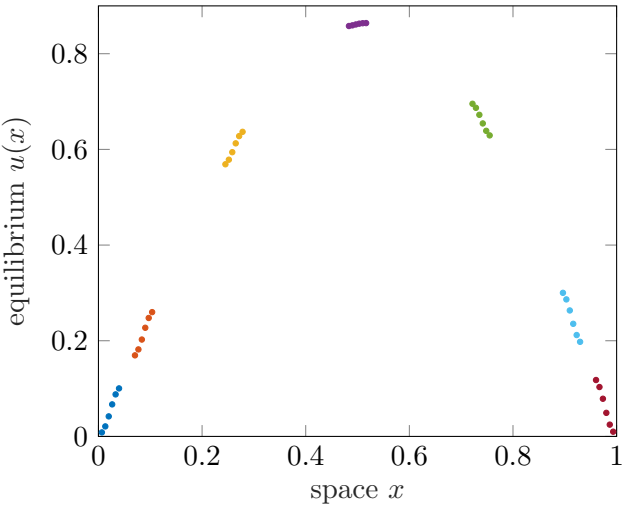


Figure 2: Equilibrium of the heterogeneous diffusion problem with forcing the same as that applied at time $t = 1$, and for relatively large $\epsilon = 0.04$ so we can see the patches. By default this code sets $\epsilon = 0.004$ whence the microscale heterogeneity and patches are tiny.

2 `EckhardtEquilib`: find an equilibrium of a 1D heterogeneous diffusion via small patches

Sections 1 and 1.2 describe details of the problem and more details of the following configuration. The aim is to find the equilibrium, Figure 2, of the forced heterogeneous system with a forcing corresponding to that applied at time $t = 1$. Computational efficiency comes from only computing the microscale heterogeneity on small spatially sparse patches, potentially much smaller than those shown in Figure 2.

First configure the patch system Establish the microscale heterogeneity has micro-period `mPeriod` on the lattice, and coefficients to match Eckhardt and Verfürth (2022) [§6.2.1].

```
clear all
global patches
%global OurCf2eps, OurCf2eps=true %option to save plots
mPeriod = 6
y = linspace(0,1,mPeriod+1)';
a = 1./(2-cos(2*pi*y(1:mPeriod)))
global microTimePeriod; microTimePeriod=0;
```

Set the number of patches, the number of periods per patch, and the spatial period ϵ, via integer $1/\epsilon$.

```
nPatch = 7
nPeriodsPatch = 1 % any integer
rEpsilon = 25 % 25 for graphic, up to 2000 say
dx = 1/(mPeriod*rEpsilon+1)
nSubP = nPeriodsPatch*mPeriod+2
```

Establish the global data struct `patches` for the microscale heterogeneous lattice diffusion system (1) solved on domain $[0, 1]$, with Chebyshev-like distribution of patches, and say fourth order interpolation to provide the edge-values. Use 'edgy' interpolation.

```
ordCC = 4
configPatches1(@heteroDiffF,[0 1],'chebyshev',nPatch ...
    ,ordCC,dx,nSubP,'EdgyInt',true,'hetCoeffs',a);
```

Set the forcing coefficients, either the original parabolic, or exp-sinusoidal. At time $t = 1$ the resultant forcing we actually apply here is simply the sum of the two components.

```
if 0 % given forcing
  patches.f1 = 2*( patches.x-patches.x.^2 );
  patches.f2 = 2*0.5+0*patches.x;
else% simple exp-sine forcing
  patches.f1 = sin(pi*patches.x).*exp(patches.x);
  patches.f2 = pi/2*sin(pi*patches.x).*exp(patches.x);
end%if
```

Find equilibrium with fsolve We seek the equilibrium for the forcing that applies at time $t = 1$ (as if that specific forcing were applying for all time). For this linear problem, it is computationally quicker using a linear solver, but `fsolve` is quicker in human time, Start the search from a zero field.

```
u = 0*patches.x;
```

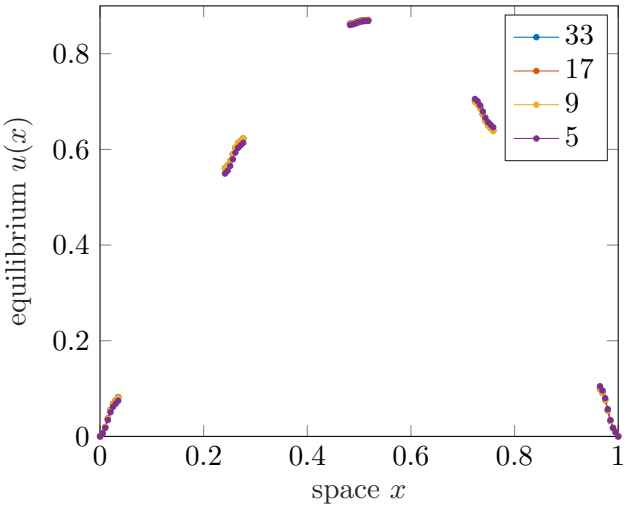
But set patch-edge values to `Nan` in order to use `patches.i` to index the interior sub-patch points as they are the variables.

```
u([1 end],:,:,:) = nan;
patches.i = find(~isnan(u));
```

Seek the equilibrium, and report the norm of the residual, via the generic patch system wrapper `theRes` (Section 11).

```
[u(patches.i),res] = fsolve(@theRes,u(patches.i));
normRes = norm(res)
```

Figure 3: Equilibrium of the heterogeneous diffusion problem for relatively large $\epsilon = 0.03$ so we can see the patches. The solution is obtained with various numbers of patches, but we only compare solutions in these five common patches.



Plot the equilibrium see Figure 2.

```
clf, plot(squeeze(patches.x),squeeze(u),'.')
xlabel('space $x$'),ylabel('equilibrium $u(x)$')
ifOurCf2tex(mfilename)%optionally save
```

3 EckhardtEquilibErrs: explore errors in equilibria of a 1D heterogeneous diffusion on small patches

Section 2 finds the equilibrium, of the forced heterogeneous system with a forcing corresponding to that applied at time $t = 1$. Computational efficiency comes from only computing the microscale heterogeneity on small spatially sparse patches. Here we explore the errors as the number N of patches increases, see Figures 3 and 4. Find mean-abs errors to be the following:

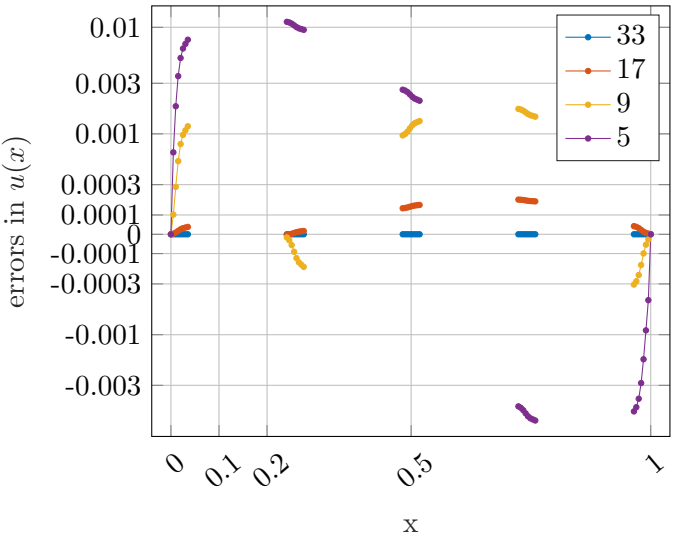


Figure 4: Errors in the equilibrium of the heterogeneous diffusion problem for relatively large $\epsilon = 0.03$. The solution is obtained with various numbers of patches, but we only plot the errors within these five common patches.

	$N =$	5	9	17	33	65
equispace	second-order	8E−3	1E−2	1E−2	4E−3	9E−4
equispace	fourth-order	2E−3	7E−4	1E−4	9E−6	5E−7
equispace	sixth-order	2E−3	2E−5	4E−7	1E−8	2E−10
chebyshev	second-order	4E−2	6E−2	3E−2	2E−2	2E−2
chebyshev	fourth-order	9E−4	3E−3	6E−4	3E−4	2E−4
chebyshev	sixth-order	9E−4	3E−5	1E−5	4E−6	1E−6
usergiven	second-order	4E−2	6E−2	3E−2	9E−3	2E−3
usergiven	fourth-order	8E−4	3E−3	6E−4	4E−5	2E−6
usergiven	sixth-order	8E−4	3E−5	1E−5	2E−7	3E−9

For 'chebyshev' this assessment of errors is a bit dodgy as it is based only on the centre and boundary patches. The 'usergiven' distribution is for overlapping patches with Chebyshev distribution of centres—a spatial 'christmas tree'[1]. Curiously, and with above caveats, here my 'smart' chebyshev is the worst, the overlapping Chebyshev is good, but *equispace appears usually the best.*

The above errors are for simple sin forcing. What if we make not so simple with exp modification of the forcing? The errors shown below are very little

[1]But the error assessment is with respect to finest patch-grid, no longer with a full domain solution

different (despite the magnitude of the solution being a little larger).

	$N=$	5	9	17	33	65
equispace	fourth-order	4E−3	7E−4	1E−4	8E−6	5E−7
chebyshev	fourth-order	7E−4	2E−3	5E−4	3E−4	1E−4
usergiven	fourth-order	2E−3	3E−3	5E−4	4E−5	2E−6

Clear, and initiate global patches. Choose the type of patch distribution to be either 'equispace', 'chebyshev', or 'usergiven'. Also set order of interpolation (fourth-order is good start).

```
clear all
global patches
%global OurCf2eps, OurCf2eps=true %option to save plots
switch 1
    case 1, Dom.type = 'equispace'
    case 2, Dom.type = 'chebyshev'
    case 3, Dom.type = 'usergiven'
    end% switch
ordInt = 4
```

First configure the patch system Establish the microscale heterogeneity has micro-period `mPeriod` on the lattice, and coefficients to match Eckhardt2210.04536 §6.2.1.

```
mPeriod = 6
z = (0.5:mPeriod)'/mPeriod;
a = 1./(2-cos(2*pi*z))
global microTimePeriod; microTimePeriod=0;
```

To use a hierarchy of patches with `nPatch` of 5, 9,17, ..., we need up to N patches plus one `dx` to fit into the domain interval. Cater for up to some full-domain simulation—can compute `log2Nmax` = 129 ($\epsilon = 0.008$) in a few seconds:

```
log2Nmax = 7 % 5 for plots, 7 for choice
nPatchMax=2^log2Nmax+1
```

Set the periodicity ϵ, and other microscale parameters.

```
nPeriodsPatch = 1 % any integer
nSubP = nPeriodsPatch*mPeriod+2 % for edgy int
epsilon = 1/(nPatchMax*nPeriodsPatch+1/mPeriod)
dx = epsilon/mPeriod
```

For various numbers of patches Choose five to be the coarsest number of patches. Want place to store common results for the solutions. Assign `Ps` to be the indices of the common patches: for equispace set to the five common patches, but for chebyshev the only common ones are the three centre and boundary-adjacent patches.

```
us=[]; xs=[]; nPs=[];
for log2N=log2Nmax:-1:2
    if log2N==log2Nmax
         Ps=linspace(1,nPatchMax ...
           ,5-2*all(Dom.type==’chebyshev’))
    else Ps=(Ps+1)/2
    end
```

Set the number of patches in $(0, 1)$:

```
    nPatch = 2^log2N+1
```

In the case of ‘usergiven’, we choose standard Chebyshev distribution of the centre of the patches, which involves overlapping of patches near the boundaries! (instead of the coded chebyshev which has a boundary layer of non-overlapping patches and a Chebyshev within the interior).

```
    if all(Dom.type==’usergiven’)
      halfWidth=dx*(nSubP-1)/2;
      X1 = 0+halfWidth; X2 = 1-halfWidth;
      Dom.X = (X1+X2)/2-(X2-X1)/2*cos(linspace(0,pi,nPatch));
    end
```

Configure the patches:

```
    configPatches1(@heteroDiffF,[0 1],Dom,nPatch ...
        ,ordInt,dx,nSubP,’EdgyInt’,true,’hetCoeffs’,a);
```

Set the forcing coefficients, either the original parabolic, or sinusoidal. At time $t = 1$ the resultant forcing we actually apply here is simply the sum of the two components.

```
    if 0 %given forcing gives exact answers for ordInt=4 !
      patches.f1 = 2*( patches.x-patches.x.^2 );
      patches.f2 = 2*0.5+0*patches.x;
    else% simple exp-sine forcing
      patches.f1 = sin(pi*patches.x).*exp(patches.x);
      patches.f2 = pi/2*sin(pi*patches.x).*exp(patches.x);
    end%if
```

Solve for steady state Set initial guess of either zero or a subsample of the next finer solution, with `NaN` to indicate patch-edge values. Index `i` are the indices of patch-interior points, and the number of unknowns is then its length.

```
    if log2N==log2Nmax
      u0 = zeros(nSubP,1,1,nPatch);
    else u0 = u0(:,:,:,1:2:end);
    end
    u0([1 end],:) = nan;
    patches.i = find(~isnan(u0));
    nVariables = numel(patches.i)
```

Solve via `fsolve` for simplicity and robustness (and using `optimoptions` to omit trace information), via the generic patch system wrapper `theRes` (Section 11).

```
    tic;
    uSoln = fsolve(@theRes,u0(patches.i) ...
        ,optimoptions('fsolve','Display','off'));
    fsolveTime = toc
```

Store the solution into the patches, and give magnitudes—Inf norm is max(abs()).

```
    normSoln = norm(uSoln,Inf)
    normResidual = norm(theRes(uSoln),Inf)
    u0(patches.i) = uSoln;
    u0 = patchEdgeInt1(u0);
    u0( 1 ,:,:, 1 ) = 0;
    u0(end,:,:,end) = 0;
```

Concatenate the solution on common patches into stores.

```
    us=cat(3,us,squeeze(u0(:,:,:,Ps)));
    xs=cat(3,xs,squeeze(patches.x(:,:,:,Ps)));
    nPs = [nPs;nPatch];
```

End loop. Check grids were aligned, then compute errors compared to the full-domain solution.

```
end%for log2N
assert(max(abs(reshape(diff(xs,1,3),[],1)))<1e-12,'x-coord failure')
errs = us-us(:,:,1);
meanAbsErrs = mean(abs(reshape(errs,[],size(us,3))))
ratioErrs = meanAbsErrs(2:end)./meanAbsErrs(1:end-1)
```

Plot solution in common patches First adjoin NaNs to separate patches, and reshape.

```
x=xs(:,:,1); u=us;
x(end+1,:)=nan; u(end+1,:)=nan;
u=reshape(u,numel(x),[]);
```

Reshape solution field.

```
figure(1),clf
plot(x(:),u,'.-'), legend(num2str(nPs))
xlabel('space $x$'),ylabel('equilibrium $u(x)$')
ifOurCf2tex([mfilename 'us'])%optionally save
```

Plot errors Use quasi-log axis to separate the errors.

```
err = u(:,1)-u;
figure(2), clf
h=plot(x(:),err,'.-'); legend(num2str(nPs))
quasiLogAxes(h,10,sqrt(prod(meanAbsErrs(2:3))))
xlabel('space $x$'), ylabel('errors in $u(x)$')
ifOurCf2tex(mfilename)%optionally save
```

4 Eckhardt2210eg1: example of 1D space-time heterogeneous diffusion via computational homogenisation with projective integration and small patches

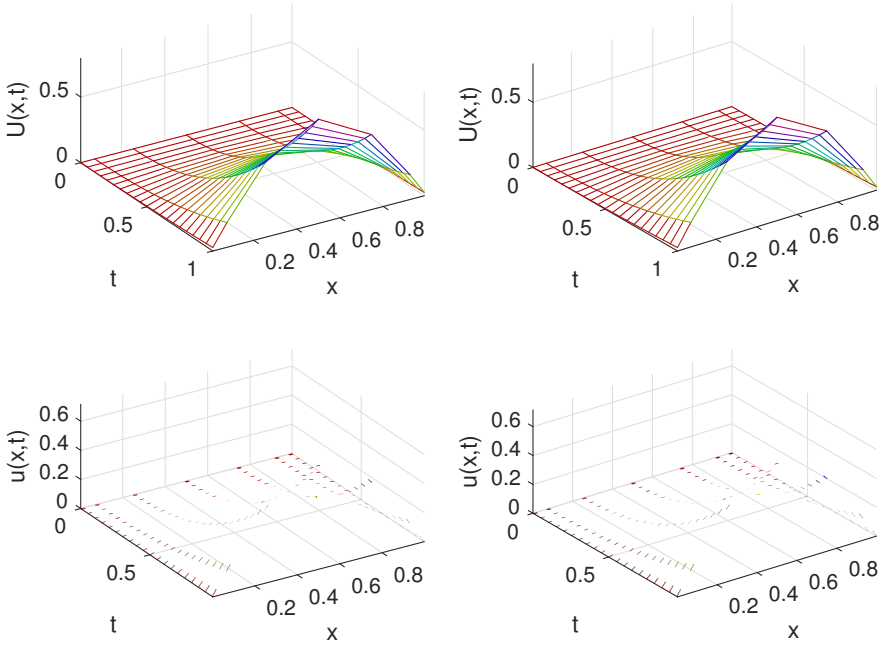
An example simulation in time generated by projective integration allied with the patch scheme applied to forced diffusion in a medium with microscale heterogeneity in both space and time. This is more-or-less the first example of Eckhardt and Verfürth (2022) [§6.2].

Suppose the spatial microscale lattice is at points x_i, with constant spacing dx. With dependent variables $u_i(t)$, simulate the microscale lattice forced diffusion system

$$\frac{\partial u_i}{\partial t} = \frac{1}{dx^2}\delta[a_{i-1/2}(t)\delta u_i] + f_i(t), \tag{2}$$

in terms of the centred difference operator δ. The system has a microscale heterogeneity via the coefficients $a_{i+1/2}$ which has given periodicity ϵ in space, and periodicity ϵ^2 in time. Figure 5 shows an example patch simulation.

Figure 5: diffusion field $u(x,t)$ of the patch scheme applied to the forced space-time heterogeneous diffusive (2). Simulate for seven patches (with a 'Chebyshev' distribution): the top stereo pair is a mesh plot of a macroscale value at the centre of each spatial patch at each projective integration time-step; the bottom stereo pair shows the corresponding tiny space-time patches in which microscale computations were carried out.



The approximate homogenised PDE is $U_t = A_0 U_{xx} + F$ with $U = 0$ at $x = 0, 1$. Its slowest mode is then $U = \sin(\pi x) e^{-A_0 \pi^2 t}$. When $A_0 = 3.3524$ as in Eckhardt then the rate of evolution is about 33 which is relatively fast on the simulation time-scale of $T = 1$. Let's slow down the dynamics by reducing diffusivities by a factor of 30, so effectively $A_0 \approx 0.1$ and $A_0 \pi^2 \approx 1$.

Also, in the microscale fluctuations change the time variation to cosine, not its square (because I cannot see the point of squaring it!).

The highest wavenumber mode on the macro-grid of patches, spacing H, is the zig-zag mode on $\dot{U}_i = A_0(U_{I+1} - 2U_I + U_{I-1})/H^2 + F_I$ which evolves like $U_I = (-1)^I e^{-\alpha t}$ for the fastest 'slow rate' of $\alpha = 4A_0^2/H^2$. When $H = 0.2$ and $A_0 \approx 0.1$ this rate is $\alpha \approx 10$.

Here use period $\epsilon = 1/100$ (so that computation completes in seconds, and because we have slowed the dynamics by 30). The patch scheme computes

only on a fraction of the spatial domain. Projective integration computes only on a fraction of the time domain determined by the 'burst length'.

4.1 Simulate heterogeneous diffusion systems

First establish the microscale heterogeneity has micro-period `mPeriod` on the spatial lattice, and coefficients inspired by Eckhardt2210.04536 §6.2. Set the phase of the heterogeneity so that each patch centre is a point of symmetry of the diffusivity. Then the heterogeneity is repeated to fill each patch. If an odd number of odd-periods in a patch, then the centre patch is a grid point of the field u, otherwise the centre patch is at a half-grid point.

```
clear all
%global OurCf2eps, OurCf2eps=true %option to save plots
mPeriod = 6
y = linspace(0,1,mPeriod+1)';
a = ( 3+cos(2*pi*y(1:mPeriod)) )/30
A0 = 1/mean(1./a) % roughly the effective diffusivity
```

The microscale diffusivity has an additional additive component of $+\frac{1}{30}\cos(2\pi t/\epsilon^2)$ which is coded into time derivative routine via global `microTimePeriod`.

Set the periodicity, via integer $1/\epsilon$, and other parameters.

```
nPeriodsPatch = 2 % any integer
rEpsilon = 100
dx = 1/(mPeriod*rEpsilon+1)
nSubP = nPeriodsPatch*mPeriod+2
tol=1e-9;
```

Set the time periodicity (global).

```
global microTimePeriod
microTimePeriod = 1/rEpsilon^2
```

Establish the global data struct `patches` for the microscale heterogeneous lattice diffusion system (2) solved on macroscale domain $[0, 1]$, with `nPatch` patches, and say fourth-order interpolation to provide the edge-values of the inter-patch coupling conditions. Distribute the patches either equispaced or chebyshev. Setting `patches.EdgyInt` true means the edge-values come from interpolating the opposite next-to-edge values of the patches (not the mid-patch values).

```
nPatch = 7
ordCC = 4
Dom = 'chebyshev'
global patches
configPatches1(@heteroDiffF,[0 1],Dom,nPatch ...
    ,ordCC,dx,nSubP,'EdgyInt',true,'hetCoeffs',a);
DX = mean(diff(squeeze(patches.x(1,1,1,:))))
```

Set the forcing coefficients as the odd-periodic extensions, accounting for roundoff error in `f2`.

```
if 0 % given forcing
  patches.f1=2*( patches.x-patches.x.^2 );
  patches.f2=2*0.5+0*patches.x;
else% simple sine forcing
  patches.f1=sin(pi*patches.x);
  patches.f2=pi/2*sin(pi*patches.x);
end%if
```

Simulate Set the initial conditions of a simulation to be zero. Mark that edge of patches are not to be used in the projective extrapolation by setting initial values to NaN.

```
u0 = 0*patches.x;
u0([1 end],:) = nan;
```

Set the desired macro- and microscale time-steps over the time domain. The macroscale step is in proportion to the effective mean diffusion time on the macroscale, here $1/(A_0\pi^2) \approx 1$ so for macro-scale error less than 1% need $\Delta t < 0.24$, so use 0.1 say.

The burst time depends upon the sub-patch effective diffusion rate β where here rate $\beta \approx \pi^2 A_0/h^2 \approx 2000$ for patch width $h \approx 0.02$: use the formula from the Manual, with some extra factor, and rounded to the nearest multiple of the time micro-periodicity.

```
ts = linspace(0,1,21)
h=(nSubP-1)*dx;
beta = pi^2*A0/h^2 % slowest rate of fast modes
burstT = 2.5*log(beta*diff(ts(1:2)))/beta
burstT = max(10,round(burstT/microTimePeriod))*microTimePeriod +1e-12
addpath('../../ProjInt')
```

Time the projective integration simulation.

```
tic
[us,tss,uss] = PIRK2(@heteroBurstF, ts, u0(:), burstT);
cputime=toc
```

Plot space-time surface of the simulation First, just a macroscale mesh plot—stereo pair.

```
xs=squeeze(patches.x);
Xs=mean(xs);
Us=squeeze(mean( reshape(us,length(ts),[],nPatch), 2,'omitnan'));
figure(1),clf
for k = 1:2, subplot(2,2,k)
  mesh(ts,Xs(:),Us')
  ylabel('x'), xlabel('t'), zlabel('U(x,t)')
  colormap(0.8*hsv), axis tight, view(62-4*k,45)
end
```

Second, plot a surface detailing the microscale bursts—stereo pair. Do not bother with the patch-edge values. Optionally save to Figs folder.

```
xs([1 end],:) = nan;
for k = 1:2, subplot(2,2,2+k)
  surf(tss,xs(:),uss',  'EdgeColor','none')
  ylabel('x'), xlabel('t'), zlabel('u(x,t)')
  colormap(0.7*hsv), axis tight, view(62-4*k,45)
end
ifOurCf2eps(mfilename)
```

4.2 `heteroBurstF()`: a burst of heterogeneous diffusion

This code integrates in time the derivatives computed by `heteroDiff` from within the patch coupling of `patchSys1`. Try `ode23`, although `ode45` may give smoother results. Sample every period of the microscale time fluctuations (or, at least, close to the period).

```
function [ts, ucts] = heteroBurstF(ti, ui, bT)
  global microTimePeriod
  [ts,ucts] = ode45( @patchSys1,ti+(0:microTimePeriod:bT),ui(:));
end
```

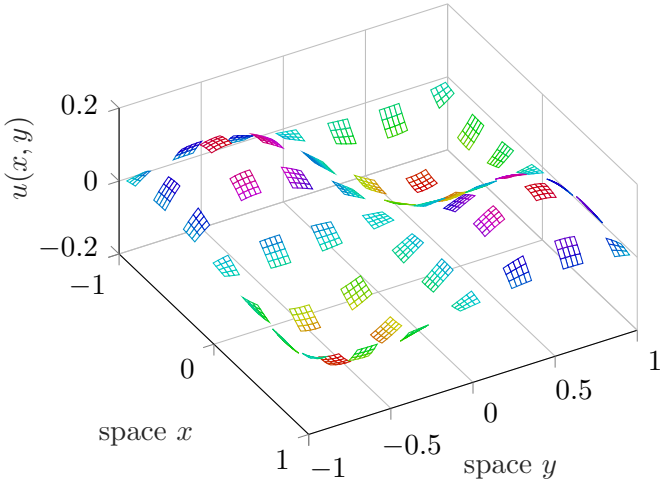


Figure 6: Equilibrium of the macroscale diffusion problem of Freese with Dirichlet zero-value boundary conditions (Section 5). The patch size is not small so we can see the patches.

5 `monoscaleDiffEquil2`: equilibrium of a 2D monoscale heterogeneous diffusion via small patches

Here we find the steady state $u(x,y)$, see Figure 6, to the heterogeneous PDE(inspired by Freese et al.[2] §5.2)

$$u_t = A(x,y)\vec{\nabla}\vec{\nabla}u - f,$$

on domain $[-1,1]^2$ with Dirichlet BCs, for coefficient pseudo-diffusion matrix

$$A := \begin{bmatrix} 2 & a \\ a & 2 \end{bmatrix} \quad \text{with } a := \operatorname{sign}(xy) \text{ or } a := \sin(\pi x)\sin(\pi y),$$

and for forcing $f(x,y)$ such that the exact equilibrium is $u = x\big(1-e^{1-|x|}\big)y\big(1-e^{1-|y|}\big)$. But for simplicity, let's obtain $u = x(1-x^2)y(1-y^2)$ for which we code f later—as determined by this Reduce algebra code.

```
on gcd; factor sin;
u:=x*(1-x^2)*y*(1-y^2);
a:=sin(pi*x)*sin(pi*y);
f:=2*df(u,x,x)+2*a*df(u,x,y)+2*df(u,y,y);
```

Clear, and initiate globals.

[2] http://arxiv.org/abs/2211.13731

```
clear all
global patches
%global OurCf2eps, OurCf2eps=true %option to save plot
```

Patch configuration Initially use 7×7 patches in the square $(-1, 1)^2$. For continuous forcing we may have small patches of any reasonable microgrid spacing—here the microgrid error dominates.

```
nPatch = 7
nSubP = 5
dx = 0.03
```

Specify some order of interpolation.

```
configPatches2(@monoscaleDiffForce2,[-1 1 -1 1],'equispace' ...
    ,nPatch ,4 ,dx ,nSubP ,'EdgyInt',true );
```

Compute the time-constant coefficient and time-constant forcing, and store them in struct `patches` for access by the microcode of Section 5.1.

```
x=patches.x;  y=patches.y;
patches.A = sin(pi*x).*sin(pi*y);
patches.fu = ...
    +2*patches.A.*(9*x.^2.*y.^2-3*x.^2-3*y.^2+1) ...
    +12*x.*y.*(x.^2+y.^2-2);
```

By construction, the PDE has analytic solution

```
uAnal = x.*(1-x.^2).*y.*(1-y.^2);
```

Solve for steady state Set initial guess of zero, with `NaN` to indicate patch-edge values. Index `i` are the indices of patch-interior points, and the number of unknowns is then its length.

```
u0 = zeros(nSubP,nSubP,1,1,nPatch,nPatch);
u0([1 end],:,:) = nan;  u0(:,[1 end],:) = nan;
patches.i = find(~isnan(u0));
nVariables = numel(patches.i)
```

Solve by iteration. Use `fsolve` for simplicity and robustness (using `optimoptions` to omit its trace information), and give magnitudes.

```
tic;
uSoln = fsolve(@theRes,u0(patches.i) ...
        ,optimoptions('fsolve','Display','off'));
solnTime = toc
normResidual = norm(theRes(uSoln))
normSoln = norm(uSoln)
normError = norm(uSoln-uAnal(patches.i))
```

Store the solution vector into the patches, and interpolate, but have not bothered to set boundary values so they stay NaN from the interpolation.

```
u0(patches.i) = uSoln;
u0 = patchEdgeInt2(u0);
```

Draw solution profile Separate patches with NaNs, then reshape arrays to suit 2D space surface plots.

```
figure(1), clf, colormap(0.8*hsv)
x(end+1,:,:)=nan;  u0(end+1,:,:)=nan;
y(:,end+1,:)=nan;  u0(:,end+1,:)=nan;
u = reshape(permute(squeeze(u0),[1 3 2 4]), [numel(x) numel(y)]);
```

Draw the patch solution surface, with boundary-values omitted as already `NaN` by not bothering to set them.

```
mesh(x(:),y(:),u'); view(60,55)
xlabel('space $x$'), ylabel('space $y$'), zlabel('$u(x,y)$')
ifOurCf2tex(mfilename)%optionally save
```

5.1 `monoscaleDiffForce2()`: microscale discretisation inside patches of forced diffusion PDE

This function codes the lattice heterogeneous diffusion of the PDE inside the patches. For 6D input arrays `u`, `x`, and `y`, computes the time derivative at each point in the interior of a patch, output in `ut`.

```
function ut = monoscaleDiffForce2(t,u,patches)
  dx = diff(patches.x(2:3));  % x space step
  dy = diff(patches.y(2:3));  % y space step
  i = 2:size(u,1)-1; % x interior points in a patch
  j = 2:size(u,2)-1; % y interior points in a patch
  ut = nan+u;         % preallocate output array
```

Set Dirichlet boundary value of zero around the square domain.

```
  u( 1 ,:,:,:, 1 ,:)=0; % left edge of left patches
  u(end,:,:,:,end,:)=0; % right edge of right patches
  u(:, 1 ,:,:,:, 1 )=0; % bottom edge of bottom patches
  u(:,end,:,:,:,end)=0; % top edge of top patches
```

Or code some function variation around the boundary, such as a function of y on the left boundary, and a (constant) function of x at the top boundary.

```
  if 0
    u(1,:,:,:,1,:)=(1+patches.y)/2; % left edge of left patches
    u(:,end,:,:,:,end)=1; % top edge of top patches
  end%if
```

Compute the time derivatives via stored forcing and coefficients. Easier to code by conflating the last four dimensions into the one `,:`.

```
  ut(i,j,:) ...
  = 2*diff(u(:,j,:),2,1)/dx^2 +2*diff(u(i,:,:),2,2)/dy^2 ...
   +2*patches.A(i,j,:).*( u(i+1,j+1,:) -u(i-1,j+1,:) ...
     -u(i+1,j-1,:) +u(i-1,j-1,:) )/(4*dx*dy) ...
   -patches.fu(i,j,:);
end%function monoscaleDiffForce2
```

6 `twoscaleDiffEquil2`: equilibrium of a 2D twoscale heterogeneous diffusion via small patches

Here we find the steady state $u(x, y)$ to the heterogeneous PDE (inspired by Freese et al.[3] §5.3.1)

$$u_t = A(x, y)\vec{\nabla}\vec{\nabla}u - f,$$

on domain $[-1, 1]^2$ with Dirichlet BCs, for coefficient 'diffusion' matrix, varying with period 2ϵ on the microscale $\epsilon = 2^{-7}$, of

$$A := \begin{bmatrix} 2 & a \\ a & 2 \end{bmatrix} \quad \text{with } a := \sin(\pi x/\epsilon)\sin(\pi y/\epsilon),$$

and for forcing $f := (x + \cos 3\pi x)y^3$.

Clear, and initiate globals.

[3] http://arxiv.org/abs/2211.13731

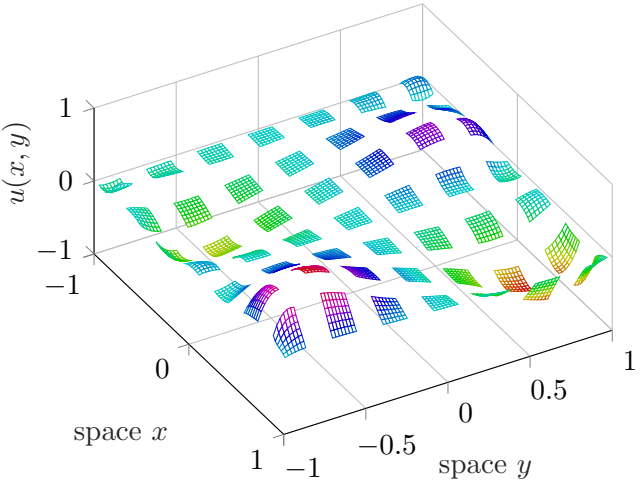


Figure 7: Equilibrium of the multiscale diffusion problem of Freese with Dirichlet zero-value boundary conditions (Section 6). The patch size is not small so we can see the patches and the sub-patch grid. The solution $u(x,y)$ is boringly smooth.

```
clear all
global patches
%global OurCf2eps, OurCf2eps=true %option to save plot
```

First establish the microscale heterogeneity has micro-period `mPeriod` on the spatial lattice. Set the phase of the heterogeneity so that each patch centre is a point of symmetry of the diffusivity. Then `configPatches2` replicates the heterogeneity to fill each patch.

```
mPeriod = 6
z = (0.5:mPeriod)'/mPeriod;
A = sin(2*pi*z).*sin(2*pi*z');
```

Set the periodicity, via ϵ, and other microscale parameters.

```
nPeriodsPatch = 1 % any integer
epsilon = 2^(-6) % 4 or 5 to see the patches
dx = (2*epsilon)/mPeriod
nSubP = nPeriodsPatch*mPeriod+2 % for edgy int
```

Patch configuration Say use 7×7 patches in $(-1,1)^2$, fourth order interpolation, and either 'equispace' or 'chebyshev':

```
nPatch = 7
configPatches2(@twoscaleDiffForce2,[-1 1],'equispace' ...
    ,nPatch ,4 ,dx ,nSubP ,'EdgyInt',true ,'hetCoeffs',A );
```

Compute the time-constant forcing, and store in struct `patches` for access by the microcode of Section 7.1.

```
x = patches.x;  y = patches.y;
patches.fu = 100*(x+cos(3*pi*x)).*y.^3;
```

Solve for steady state Set initial guess of zero, with `NaN` to indicate patch-edge values. Index `i` are the indices of patch-interior points, and the number of unknowns is then its length.

```
u0 = zeros(nSubP,nSubP,1,1,nPatch,nPatch);
u0([1 end],:,:) = nan;  u0(:,[1 end],:) = nan;
patches.i = find(~isnan(u0));
nVariables = numel(patches.i)
```

Solve by iteration. Use `fsolve` for simplicity and robustness (and using `optimoptions` to omit trace information), via the generic patch system wrapper `theRes` (Section 11), and give magnitudes.

```
tic;
uSoln = fsolve(@theRes,u0(patches.i) ...
        ,optimoptions('fsolve','Display','off'));
solveTime = toc
normResidual = norm(theRes(uSoln))
normSoln = norm(uSoln)
```

Store the solution vector into the patches, and interpolate, but have not bothered to set boundary values so they stay NaN from the interpolation.

```
u0(patches.i) = uSoln;
u0 = patchEdgeInt2(u0);
```

Draw solution profile Separate patches with NaNs, then reshape arrays to suit 2D space surface plots.

```
figure(1), clf, colormap(0.8*hsv)
x(end+1,:,:)=nan;  u0(end+1,:,:)=nan;
y(:,end+1,:)=nan;  u0(:,end+1,:)=nan;
u = reshape(permute(squeeze(u0),[1 3 2 4]), [numel(x) numel(y)]);
```

Draw the patch solution surface, with boundary-values omitted as already `NaN` by not bothering to set them.

```
mesh(x(:),y(:),u'); view(60,55)
xlabel('space $x$'), ylabel('space $y$'), zlabel('$u(x,y)$')
ifOurCf2tex(mfilename)%optionally save
```

6.1 `twoscaleDiffForce2()`: microscale discretisation inside patches of forced diffusion PDE

This function codes the lattice heterogeneous diffusion of the PDE inside the patches. For 6D input arrays `u`, `x`, and `y`, computes the time derivative at each point in the interior of a patch, output in `ut`.

```
function ut = twoscaleDiffForce2(t,u,patches)
  dx = diff(patches.x(2:3));  % x space step
  dy = diff(patches.y(2:3));  % y space step
  i = 2:size(u,1)-1; % x interior points in a patch
  j = 2:size(u,2)-1; % y interior points in a patch
  ut = nan+u;          % preallocate output array
```

Set Dirichlet boundary value of zero around the square domain.

```
  u( 1 ,:,:,:, 1 ,:)=0; % left edge of left patches
  u(end,:,:,:,end,:)=0; % right edge of right patches
  u(:, 1 ,:,:,:, 1 )=0; % bottom edge of bottom patches
  u(:,end,:,:,:,end)=0; % top edge of top patches
```

Compute the time derivatives via stored forcing and coefficients. Easier to code by conflating the last four dimensions into the one `,:`.

```
  ut(i,j,:) ...
  = 2*diff(u(:,j,:),2,1)/dx^2 +2*diff(u(i,:,:),2,2)/dy^2 ...
   +2*patches.cs(i,j).*( u(i+1,j+1,:) -u(i-1,j+1,:) ...
     -u(i+1,j-1,:) +u(i-1,j-1,:) )/(4*dx*dy) ...
   -patches.fu(i,j,:);
end%function twoscaleDiffForce2
```

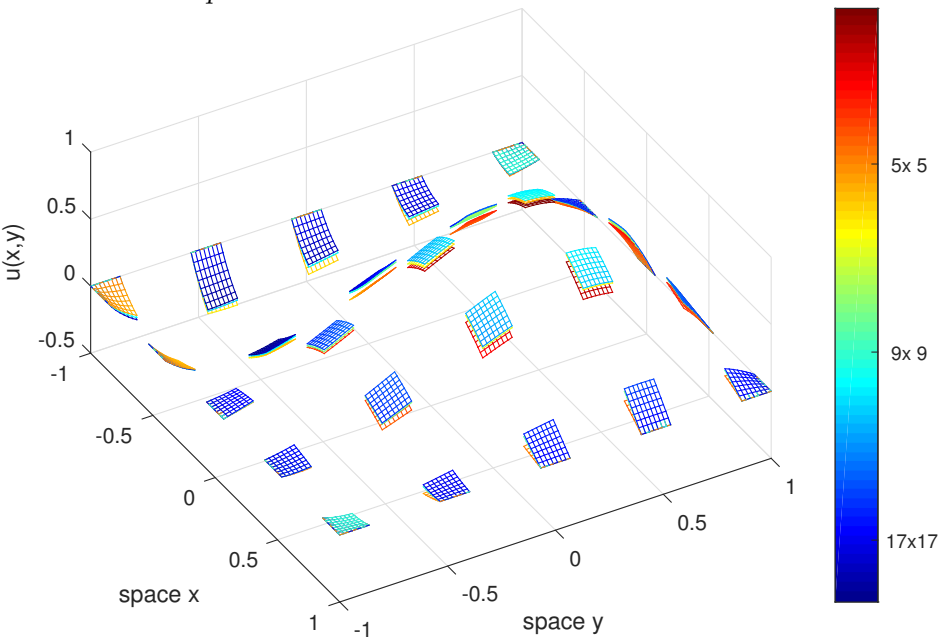
7 `twoscaleDiffEquil2Errs`: errors in equilibria of a 2D twoscale heterogeneous diffusion via small patches

Here we find the steady state $u(x,y)$ to the heterogeneous PDE (inspired by Freese et al.[4] §5.3.1)

$$u_t = A(x,y)\vec{\nabla}\vec{\nabla}u + f,$$

[4] http://arxiv.org/abs/2211.13731

Figure 8: For various numbers of patches as indicated on the colorbar, plot the equilibrium of the multiscale diffusion problem of Freese with Dirichlet zero-value boundary conditions (Section 7). We only compare solutions only in these 25 common patches.



on domain $[-1,1]^2$ with Dirichlet BCs, for coefficient 'diffusion' matrix, varying with some microscale period ϵ (here $\epsilon \approx 0.24, 0.12, 0.06, 0.03$), of

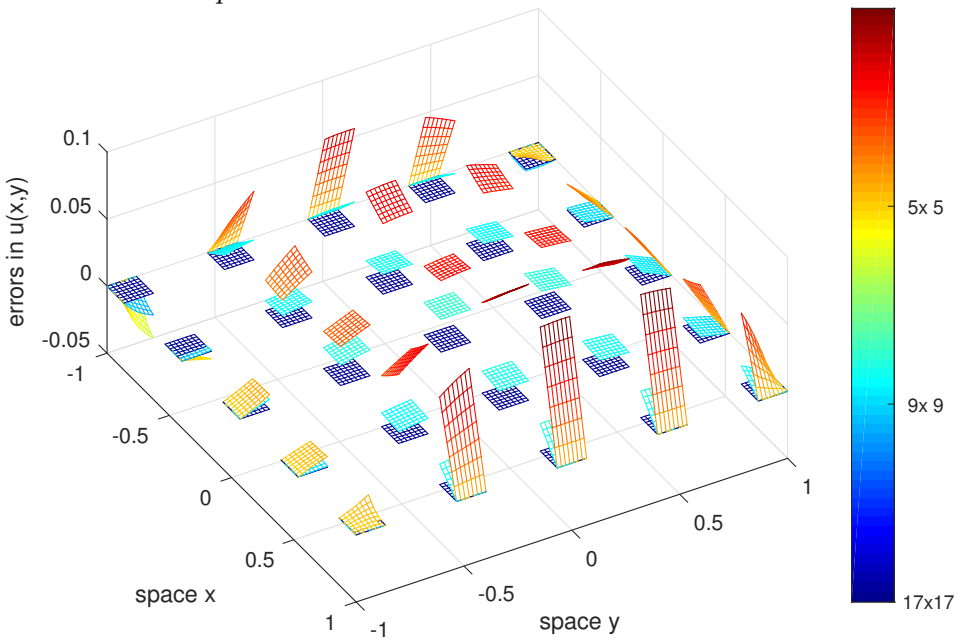
$$A := \begin{bmatrix} 2 & a \\ a & 2 \end{bmatrix} \quad \text{with } a := \sin(\pi x/\epsilon)\sin(\pi y/\epsilon),$$

and for forcing $f := 10(x + y + \cos \pi x)$ (for which the solution has magnitude up to one).[5]

Here we explore the errors for increasing number N of patches (in both directions). Find mean-abs errors to be the following (for different orders of

[5]Freese et al. had forcing $f := (x + \cos 3\pi x)y^3$, but here we want smoother forcing so we get meaningful results in a minute or two computation.[6] For the same reason we do not invoke their smaller $\epsilon \approx 0.01$.

Figure 9: For various numbers of patches as indicated on the colorbar, plot the equilibrium of the multiscale diffusion problem of Freese with Dirichlet zero-value boundary conditions (Section 7). We only compare solutions only in these 25 common patches.



interpolation and patch distribution):

N	5	9	17	33
equispace, 2nd-order	6E−2	3E−2	1E−2	3E−3
equispace, 4th-order	3E−2	8E−3	7E−4	7E−5
chebyshev, 4th-order	1E−2	2E−2	6E−3	2E−3
usergiven, 4th-order	1E−2	2E−2	4E−3	n/a
equispace, 6th-order	3E−2	1E−3	1E−4	2E−5

Script start Clear, and initiate global patches. Choose the type of patch distribution to be either 'equispace', 'chebyshev', or 'usergiven'. Also set order of interpolation (fourth-order is good start).

```
clear all
global patches
%global OurCf2eps, OurCf2eps=true %option to save plot
```

```
switch 1
    case 1, Dom.type = 'equispace'
    case 2, Dom.type = 'chebyshev'
    case 3, Dom.type = 'usergiven'
end% switch
ordInt = 4
```

First configure the patch system Establish the microscale heterogeneity has micro-period `mPeriod` on the spatial lattice. Then `configPatches2` replicates the heterogeneity as needed to fill each patch.

```
mPeriod = 6
z = (0.5:mPeriod)'/mPeriod;
A = sin(2*pi*z).*sin(2*pi*z');
```

To use a hierarchy of patches with `nPatch` of 5, 9, 17, ..., we need up to N patches plus one `dx` to fit into the domain interval. Cater for up to some full-domain simulation—can compute `log2Nmax` $= 5$ ($\epsilon = 0.06$) within minutes:

```
log2Nmax = 4 % >2 up to 6 OKish
nPatchMax=2^log2Nmax+1
```

Set the periodicity ϵ, and other microscale parameters.

```
nPeriodsPatch = 1 % any integer
nSubP = nPeriodsPatch*mPeriod+2 % for edgy int
epsilon = 2/(nPatchMax*nPeriodsPatch+1/mPeriod)
dx = epsilon/mPeriod
```

For various numbers of patches Choose five patches to be the coarsest number of patches. Define variables to store common results for the solutions from differing patches. Assign `Ps` to be the indices of the common patches: for equispace set to the five common patches, but for 'chebyshev' the only common ones are the three centre and boundary-adjacent patches.

```
us=[]; xs=[]; ys=[]; nPs=[];
for log2N=log2Nmax:-1:2
    if log2N==log2Nmax
        Ps=linspace(1,nPatchMax ...
          ,5-2*all(Dom.type=='chebyshev'))
    else Ps=(Ps+1)/2
    end
```

Set the number of patches in $(-1, 1)$:

```
148     nPatch = 2^log2N+1
```

In the case of 'usergiven', we set the standard Chebyshev distribution of the patch-centres, which involves overlapping of patches near the boundaries! (instead of the coded chebyshev which has boundary layers of abutting patches, and non-overlapping Chebyshev between the boundary layers).

```
159     if all(Dom.type=='usergiven')
160       halfWidth = dx*(nSubP-1)/2;
161       X1 = -1+halfWidth;  X2 = 1-halfWidth;
162       Dom.X = (X1+X2)/2-(X2-X1)/2*cos(linspace(0,pi,nPatch));
163       Dom.Y = Dom.X;
164     end
```

Configure the patches:

```
170     configPatches2(@twoscaleDiffForce2,[-1 1],Dom,nPatch  ...
171         ,ordInt ,dx ,nSubP ,'EdgyInt',true ,'hetCoeffs',A );
```

Compute the time-constant forcing, and store in struct `patches` for access by the microcode of Section 7.1.

```
179     if 1
180       patches.fu = 10*(patches.x+cos(pi*patches.x)+patches.y);
181     else patches.fu = 8+0*patches.x+0*patches.y;
182     end
```

Solve for steady state Set initial guess of either zero or a subsample of the previous, next-finer, solution. `NaN` indicates patch-edge values. Index `i` are the indices of patch-interior points, and the number of unknowns is then its length.

```
193     if log2N==log2Nmax
194          u0 = zeros(nSubP,nSubP,1,1,nPatch,nPatch);
195     else u0 = u0(:,:,:,:,1:2:end,1:2:end);
196     end
197     u0([1 end],:,:) = nan;  u0(:,[1 end],:) = nan;
198     patches.i = find(~isnan(u0));
199     nVariables = numel(patches.i)
```

First try to solve via iterative solver `bicgstab`, via the generic patch system wrapper `theRes` (Section 11).

```
    tic;
    maxIt = ceil(nVariables/10);
    rhsb = theRes( zeros(size(patches.i)) );
    [uSoln,flag] = bicgstab(@(u) rhsb-theRes(u),rhsb ...
                   ,1e-9,maxIt,[],[],u0(patches.i));
    bicgTime = toc
```

However, the above often fails (and `fsolve` sometimes takes too long here), so then try a preconditioned version of `bicgstab`. The preconditioner is derived from the Jacobian which is expensive to find (four minutes for $N = 33$, one hour for $N = 65$), but we do so as follows.

```
    if flag>0, disp('**** bicg failed, trying ILU preconditioner')
        disp(['Computing Jacobian: wait roughly ' ...
              num2str(nPatch^4/4500,2) ' secs'])
        tic
        Jac=sparse(nVariables,nVariables);
        for j=1:nVariables
            Jac(:,j)=sparse( rhsb-theRes((1:nVariables)'==j) );
        end
        formJacTime=toc
```

Compute an incomplete LU-factorization, and use it as preconditioner to `bicgstab`.

```
        tic
        [L,U] = ilu(Jac,struct('type','ilutp','droptol',1e-4));
        LUfillFactor = (nnz(L)+nnz(U))/nnz(Jac)
        [uSoln,flag] = bicgstab(@(u) rhsb-theRes(u),rhsb ...
                   ,1e-9,maxIt,L,U,u0(patches.i));
        precondSolveTime=toc
        assert(flag==0,'preconditioner fails bicgstab. Lower droptol?
    end%if flag
```

Store the solution into the patches, and give magnitudes—Inf norm is max(abs()).

```
    normResidual = norm(theRes(uSoln),Inf)
    normSoln = norm(uSoln,Inf)
    u0(patches.i) = uSoln;
    u0 = patchEdgeInt2(u0);
    u0( 1 ,:,:,:, 1 ,:)=0; % left edge of left patches
```

```
256      u0(end,:,:,:,end,:)=0; % right edge of right patches
257      u0(:, 1 ,:,:,:, 1 )=0; % bottom edge of bottom patches
258      u0(:,end,:,:,:,end)=0; % top edge of top patches
259      assert(normResidual<1e-5,'poor--bad solution found')
```

Concatenate the solution on common patches into stores.

```
265      us=cat(5,us,squeeze(u0(:,:,:,:,Ps,Ps)));
266      xs=cat(3,xs,squeeze(patches.x(:,:,:,:,Ps,:)));
267      ys=cat(3,ys,squeeze(patches.y(:,:,:,:,:,Ps)));
268      nPs = [nPs;nPatch];
```

End loop. Check micro-grids are aligned, then compute errors compared to the full-domain solution (or the highest resolution solution for the case of 'usergiven').

```
277  end%for log2N
278  assert(max(abs(reshape(diff(xs,1,3),[],1)))<1e-12,'x-coord failure')
279  assert(max(abs(reshape(diff(ys,1,3),[],1)))<1e-12,'y-coord failure')
280  errs = us-us(:,:,:,:,1);
281  meanAbsErrs = mean(abs(reshape(errs,[],size(us,5))))
282  ratioErrs = meanAbsErrs(2:end)./meanAbsErrs(1:end-1)
```

Plot solution in common patches First reshape arrays to suit 2D space surface plots, inserting nans to separate patches.

```
294  x = xs(:,:,1); y = ys(:,:,1); u=us;
295  x(end+1,:)=nan;   y(end+1,:)=nan;
296  u(end+1,:,:)=nan; u(:,end+1,:)=nan;
297  u = reshape(permute(u,[1 3 2 4 5]),numel(x),numel(y),[]);
```

Plot the patch solution surfaces, with colour offset between surfaces (best if u-field has a range of one): blues are the full-domain solution, reds the coarsest patches.

```
305  figure(1), clf, colormap(jet)
306  for p=1:size(u,3)
307       mesh(x(:),y(:),u(:,:,p)',p+u(:,:,p)');
308       hold on;
309  end, hold off
310  view(60,55)
```

```
colorbar('Ticks',1:size(u,3) ...
    ,'TickLabels',[num2str(nPs) ['x';'x';'x'] num2str(nPs)]);
xlabel('space x'), ylabel('space y'), zlabel('u(x,y)')
ifOurCf2eps([mfilename 'us'])%optionally save
```

Plot error surfaces Plot the error surfaces, with colour offset between surfaces (best if u-field has a range of one): dark blue is the full-domain zero error, reds the coarsest patches.

```
err=u(:,:,1)-u;
maxAbsErr=max(abs(err(:)));
figure(2), clf, colormap(jet)
for p=1:size(u,3)
     mesh(x(:),y(:),err(:,:,p)',p+err(:,:,p)'/maxAbsErr);
     hold on;
end, hold off
view(60,55)
colorbar('Ticks',1:size(u,3) ...
    ,'TickLabels',[num2str(nPs) ['x';'x';'x'] num2str(nPs)]);
xlabel('space x'), ylabel('space y')
zlabel('errors in u(x,y)')
ifOurCf2eps(mfilename)%optionally save
```

7.1 `twoscaleDiffForce2()`: microscale discretisation inside patches of forced diffusion PDE

This function codes the lattice heterogeneous diffusion of the PDE inside the patches. For 6D input arrays `u`, `x`, and `y`, computes the time derivative at each point in the interior of a patch, output in `ut`.

```
function ut = twoscaleDiffForce2(t,u,patches)
  dx = diff(patches.x(2:3));  % x space step
  dy = diff(patches.y(2:3));  % y space step
  i = 2:size(u,1)-1; % x interior points in a patch
  j = 2:size(u,2)-1; % y interior points in a patch
  ut = nan+u;         % preallocate output array
```

Set Dirichlet boundary value of zero around the square domain.

```
  u( 1 ,:,:,:, 1 ,:)=0; % left edge of left patches
  u(end,:,:,:,end,:)=0; % right edge of right patches
```

```
  u(:, 1 ,:,:,:, 1 )=0; % bottom edge of bottom patches
  u(:,end,:,:,:,end)=0; % top edge of top patches
```

Compute the time derivatives via stored forcing and coefficients. Easier to code by conflating the last four dimensions into the one `,:`.

```
  ut(i,j,:) ...
  = 2*diff(u(:,j,:),2,1)/dx^2 +2*diff(u(i,:,:),2,2)/dy^2 ...
   +2*patches.cs(i,j).*( u(i+1,j+1,:) -u(i-1,j+1,:) ...
     -u(i+1,j-1,:) +u(i-1,j-1,:) )/(4*dx*dy) ...
   +patches.fu(i,j,:);
end%function twoscaleDiffForce2
```

8 `abdulleDiffEquil2`: equilibrium of a 2D multiscale heterogeneous diffusion via small patches

Here we find the steady state $u(x, y)$ to the heterogeneous PDE (inspired by Abdulle, Arjmand, and Paganoni 2020, §5.1)

$$u_t = \vec{\nabla} \cdot [a(x, y)\vec{\nabla} u] + 10,$$

on square domain $[0, 1]^2$ with zero-Dirichlet BCs, for coefficient 'diffusion' matrix, varying with period ϵ of (their (45))

$$a := \frac{2 + 1.8 \sin 2\pi x/\epsilon}{2 + 1.8 \cos 2\pi y/\epsilon} + \frac{2 + \sin 2\pi y/\epsilon}{2 + 1.8 \cos 2\pi x/\epsilon}.$$

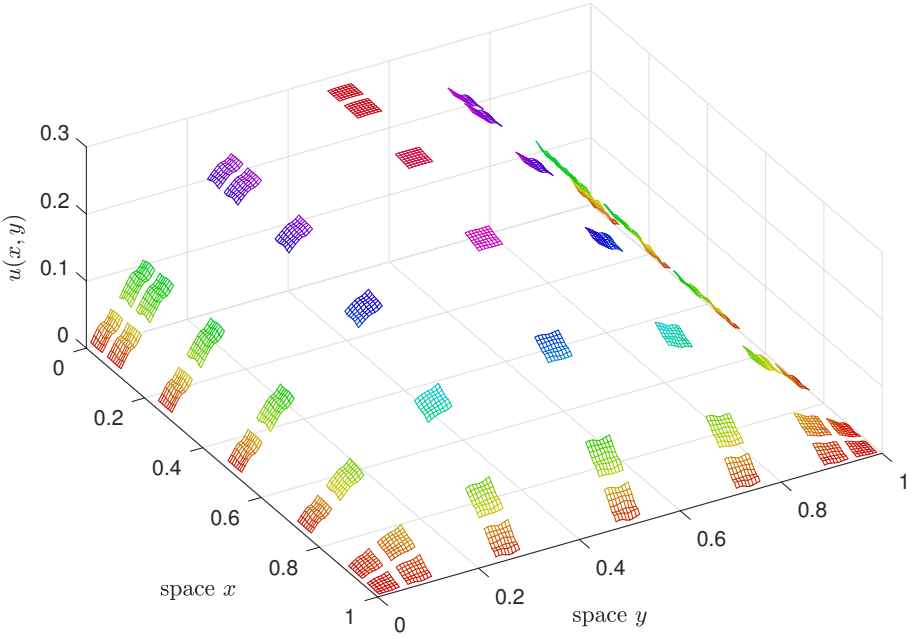
Figure 10 shows solutions have some nice microscale wiggles reflecting the heterogeneity.

Clear, and initiate globals.

```
clear all
global patches
%global OurCf2eps, OurCf2eps=true %option to save plot
```

First establish the microscale heterogeneity has micro-period `mPeriod` on the spatial micro-grid lattice. Then `configPatches2` replicates the heterogeneity to fill each patch. (These diffusion coefficients should really recognise the half-grid-point shifts, but let's not bother.)

Figure 10: Equilibrium of the macroscale diffusion problem of Abdulle with boundary conditions of Dirichlet zero-value except for $x = 0$ which is Neumann (Section 8). Here the patches have a Chebyshev-like spatial distribution. The patch size is chosen large enough to see within.




```
mPeriod = 6
x = (0.5:mPeriod)'/mPeriod;  y=x';
a = (2+1.8*sin(2*pi*x))./(2+1.8*sin(2*pi*y)) ...
   +(2+    sin(2*pi*y))./(2+1.8*sin(2*pi*x));
diffusivityRange = [min(a(:)) max(a(:))]
```

Set the periodicity ϵ, here big enough so we can see the patches, and other microscale parameters.

```
epsilon = 0.04
dx = epsilon/mPeriod
nPeriodsPatch = 1 % any integer
nSubP = nPeriodsPatch*mPeriod+2 % when edgy int
```

Patch configuration Choose either Dirichlet (default) or Neumann on the left boundary in coordination with micro-code in Section 8.1

```
78 Dom.bcOffset = zeros(2);
79 if 1, Dom.bcOffset(1)=0.5; end% left Neumann
```

Say use 7×7 patches in $(0, 1)^2$, fourth order interpolation, and either 'equispace' or 'chebyshev':

```
86 nPatch = 7
87 Dom.type='chebyshev';
88 configPatches2(@abdulleDiffForce2,[0 1],Dom ...
89     ,nPatch ,4 ,dx ,nSubP ,'EdgyInt',true ,'hetCoeffs',a );
```

Solve for steady state Set initial guess of zero, with `NaN` to indicate patch-edge values. Index `i` are the indices of patch-interior points, and the number of unknowns is then its length.

```
102 u0 = zeros(nSubP,nSubP,1,1,nPatch,nPatch);
103 u0([1 end],:,:) = nan;  u0(:,[1 end],:) = nan;
104 patches.i = find(~isnan(u0));
105 nVariables = numel(patches.i)
```

Solve by iteration. Use `fsolve` for simplicity and robustness (and using `optimoptions` to omit trace information), via the generic patch system wrapper `theRes` (Section 11), and give magnitudes.

```
114 tic;
115 uSoln = fsolve(@theRes,u0(patches.i) ...
116         ,optimoptions('fsolve','Display','off'));
117 solnTime = toc
118 normResidual = norm(theRes(uSoln))
119 normSoln = norm(uSoln)
```

Store the solution vector into the patches, and interpolate, but have not bothered to set boundary values so they stay NaN from the interpolation.

```
127 u0(patches.i) = uSoln;
128 u0 = patchEdgeInt2(u0);
```

Draw solution profile Separate patches with NaNs, then reshape arrays to suit 2D space surface plots.

```
figure(1), clf, colormap(0.8*hsv)
patches.x(end+1,:,:)=nan;  u0(end+1,:,:)=nan;
patches.y(:,end+1,:)=nan;  u0(:,end+1,:)=nan;
u = reshape(permute(squeeze(u0),[1 3 2 4]) ...
    , [numel(patches.x) numel(patches.y)]);
```

Draw the patch solution surface, with boundary-values omitted as already `NaN` by not bothering to set them.

```
mesh(patches.x(:),patches.y(:),u'); view(60,55)
xlabel('space $x$'), ylabel('space $y$'), zlabel('$u(x,y)$')
ifOurCf2eps(mfilename) %optionally save plot
```

8.1 `abdulleDiffForce2()`: microscale discretisation inside patches of forced diffusion PDE

This function codes the lattice heterogeneous diffusion of the PDE inside the patches. For 6D input arrays `u`, `x`, and `y`, computes the time derivative at each point in the interior of a patch, output in `ut`.

```
function ut = abdulleDiffForce2(t,u,patches)
  dx = diff(patches.x(2:3));  % x space step
  dy = diff(patches.y(2:3));  % y space step
  i = 2:size(u,1)-1; % x interior points in a patch
  j = 2:size(u,2)-1; % y interior points in a patch
  ut = nan+u;         % preallocate output array
```

Set Dirichlet boundary value of zero around the square domain, but also cater for zero Neumann condition on the left boundary.

```
  u( 1 ,:,:,:, 1 ,:)=0; % left edge of left patches
  u(end,:,:,:,end,:)=0; % right edge of right patches
  u(:, 1 ,:,:,:, 1 )=0; % bottom edge of bottom patches
  u(:,end,:,:,:,end)=0; % top edge of top patches
  if 1, u(1,:,:,:,1,:)=u(2,:,:,:,1,:); end% left Neumann
```

Compute the time derivatives via stored forcing and coefficients. Easier to code by conflating the last four dimensions into the one `,:`.

```
  ut(i,j,:) = diff(patches.cs(:,j).*diff(u(:,j,:)))/dx^2 ...
      + diff(patches.cs(i,:).*diff(u(i,:,:),1,2),1,2)/dy^2 ...
      + 10;
end%function abdulleDiffForce2
```

9 `randAdvecDiffEquil2`: equilibrium of a 2D random heterogeneous advection-diffusion via small patches

Here we find the steady state $u(x,y)$ of the heterogeneous PDE (inspired by Bonizzoni et al.[7] §6.2)

$$u_t = \mu_1 \nabla^2 u - (\cos\mu_2, \sin\mu_2)\cdot\vec{\nabla}u - u + f\,,$$

on domain $[0,1]^2$ with Neumann boundary conditions, for microscale random pseudo-diffusion and pseudo-advection coefficients, $\mu_1(x,y) \in [0.01, 0.1]$[8] and $\mu_2(x,y) \in [0, 2\pi)$, and for forcing

$$f(x,y) := \exp\left[-\frac{(x-\mu_3)^2 + (y-\mu_4)^2}{\mu_5^2}\right],$$

smoothly varying in space for fixed $\mu_3, \mu_4 \in [0.25, 0.75]$ and $\mu_5 \in [0.1, 0.25]$. The above system is dominantly diffusive for lengths scales $\ell < 0.01 = \min\mu_1$. Due to the randomness, we get different solutions each execution of this code. Figure 11 plots one example. A physical interpretation of the solution field is confounded because the problem is pseudo-advection-diffusion due to the varying coefficients being outside the $\vec{\nabla}$ operator.

Clear, and initiate globals.

```
clear all
global patches
%global OurCf2eps, OurCf2eps=true %option to save plot
```

First establish the microscale heterogeneity has micro-period `mPeriod` on the spatial lattice. Then `configPatches2` replicates the heterogeneity to fill each patch.

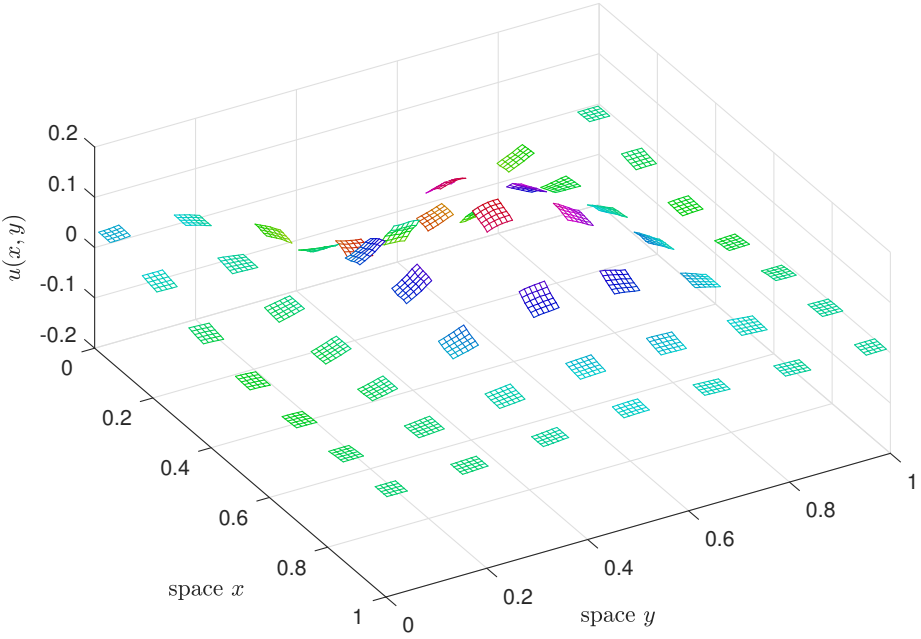
```
mPeriod = 4
mu1 = 0.01*10.^rand(mPeriod)
mu2 = 2*pi*rand(mPeriod)
cs = cat(3,mu1,cos(mu2),sin(mu2));
meanDiffAdvec=squeeze(mean(mean(cs)))
```

Set the periodicity ϵ, here big enough so we can see the patches, and other microscale parameters.

[7] http://arxiv.org/abs/2211.15221

[8] More interesting microscale structure arises here for μ_1 a factor of three smaller.

Figure 11: Equilibrium of the macroscale diffusion problem of Bonizzoni et al. with Neumann boundary conditions of zero (Section 9). Here the patches have a equispaced spatial distribution. The microscale periodicity, and hence the patch size, is chosen large enough to see within.




```
epsilon = 0.04
dx = epsilon/mPeriod
nPeriodsPatch = 1 % any integer
nSubP = nPeriodsPatch*mPeriod+2 % for edgy int
```

Patch configuration Say use 7×7 patches in $(0,1)^2$, fourth order interpolation, either 'equispace' or 'chebyshev', and the offset for Neumann boundary conditions:

```
nPatch = 7
Dom.type= 'equispace';
Dom.bcOffset = 0.5;
configPatches2(@randAdvecDiffForce2,[0 1],Dom ...
    ,nPatch ,4 ,dx ,nSubP ,'EdgyInt',true ,'hetCoeffs',cs );
```

Compute the time-constant forcing, and store in struct `patches` for access by

the microcode of Section 9.1.

```
mu = [ 0.25+0.5*rand(1,2) 0.1+0.15*rand ]
patches.fu = exp(-((patches.x-mu(1)).^2 ...
                   +(patches.y-mu(2)).^2)/mu(3)^2);
```

Solve for steady state Set initial guess of zero, with `NaN` to indicate patch-edge values. Index `i` are the indices of patch-interior points, store in global patches for access by `theRes`, and the number of unknowns is then its number of elements.

```
u0 = zeros(nSubP,nSubP,1,1,nPatch,nPatch);
u0([1 end],:,:) = nan;  u0(:,[1 end],:) = nan;
patches.i = find(~isnan(u0));
nVariables = numel(patches.i)
```

Solve by iteration. Use `fsolve` for simplicity and robustness (and using `optimoptions` to omit trace information), via the generic patch system wrapper `theRes` (Section 11).

```
tic;
uSoln = fsolve(@theRes,u0(patches.i) ...
        ,optimoptions('fsolve','Display','off'));
solnTime = toc
normResidual = norm(theRes(uSoln))
normSoln = norm(uSoln)
```

Store the solution vector into the patches, and interpolate, but have not bothered to set boundary values so they stay NaN from the interpolation.

```
u0(patches.i) = uSoln;
u0 = patchEdgeInt2(u0);
```

Draw solution profile Separate patches with NaNs, then reshape arrays to suit 2D space surface plots.

```
figure(1), clf, colormap(0.8*hsv)
patches.x(end+1,:,:)=nan;  u0(end+1,:,:)=nan;
patches.y(:,end+1,:)=nan;  u0(:,end+1,:)=nan;
u = reshape(permute(squeeze(u0),[1 3 2 4]) ...
    , [numel(patches.x) numel(patches.y)]);
```

Draw the patch solution surface, with boundary-values omitted as already `NaN` by not bothering to set them.

```
mesh(patches.x(:),patches.y(:),u'); view(60,55)
xlabel('space $x$'), ylabel('space $y$'), zlabel('$u(x,y)$')
ifOurCf2eps(mfilename) %optionally save plot
```

9.1 `randAdvecDiffForce2()`: microscale discretisation inside patches of forced diffusion PDE

This function codes the lattice heterogeneous diffusion of the PDE inside the patches. For 6D input arrays `u`, `x`, and `y`, computes the time derivative at each point in the interior of a patch, output in `ut`.

```
function ut = randAdvecDiffForce2(t,u,patches)
  dx = diff(patches.x(2:3));  % x space step
  dy = diff(patches.y(2:3));  % y space step
  i = 2:size(u,1)-1; % x interior points in a patch
  j = 2:size(u,2)-1; % y interior points in a patch
  ut = nan+u;         % preallocate output array
```

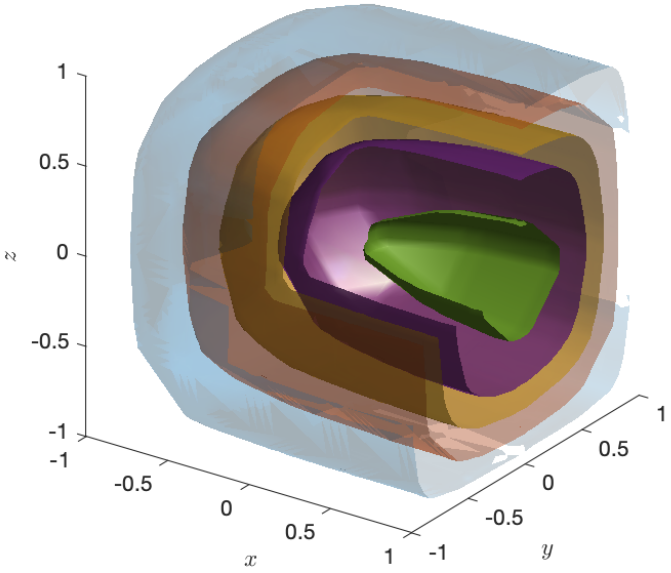
Set Neumann boundary condition of zero derivative around the square domain: that is, the edge value equals the next-to-edge value.

```
  u( 1 ,:,:,:, 1 ,:)=u(  2  ,:,:,:, 1 ,:); % left edge of left patche
  u(end,:,:,:,end,:)=u(end-1,:,:,:,end,:); % right edge of right patc
  u(:, 1 ,:,:,:, 1 )=u(:,  2  ,:,:,:, 1 ); % bottom edge of bottom pa
  u(:,end,:,:,:,end)=u(:,end-1,:,:,:,end); % top edge of top patches
```

Compute the time derivatives via stored forcing and coefficients. Easier to code by conflating the last four dimensions into the one `,:`.

```
  ut(i,j,:) ...
  = patches.cs(i,j,1).*(diff(u(:,j,:),2,1)/dx^2 ...
                        +diff(u(i,:,:),2,2)/dy^2)...
   -patches.cs(i,j,2).*(u(i+1,j,:)-u(i-1,j,:))/(2*dx) ...
   -patches.cs(i,j,3).*(u(i,j+1,:)-u(i,j-1,:))/(2*dy) ...
   -u(i,j,:) +patches.fu(i,j,:);
end%function randAdvecDiffForce2
```

Figure 12: macroscale of the random heterogeneous diffusion in 3D with boundary conditions of zero on all faces except for the Neumann condition on $x = 1$ (Section 10). The small patches are equispaced in space.



10 `homoDiffBdryEquil3`: equilibrium via computational homogenisation of a 3D heterogeneous diffusion on small patches

Find the equilibrium of a forced heterogeneous diffusion in 3D space on 3D patches as an example application. Boundary conditions are Neumann on the right face of the cube, and Dirichlet on the other faces. Figure 12 shows five isosurfaces of the 3D solution field.

Clear variables, and establish globals.

```
clear all
global patches
%global OurCf2eps, OurCf2eps=true %option to save plots
```

Set random heterogeneous diffusivities of random (small) period in each of the three directions. Crudely normalise by the harmonic mean so the decay time scale is roughly one.

```
mPeriod = randi([2 3],1,3)
cDiff = exp(0.3*randn([mPeriod 3]));
cDiff = cDiff*mean(1./cDiff(:))
```

Configure the patch scheme with some arbitrary choices of cubic domain, patches, and micro-grid spacing 0.05. Use high order interpolation as few patches in each direction. Configure for Dirichlet boundaries except for Neumann on the right x-face.

```
nSubP = mPeriod+2;
nPatch = 5;
Dom.type = 'equispace';
Dom.bcOffset = zeros(2,3);  Dom.bcOffset(2) = 0.5;
configPatches3(@microDiffBdry3, [-1 1], Dom ...
    , nPatch, 0, 0.05, nSubP, 'EdgyInt',true  ...
    ,'hetCoeffs',cDiff );
```

Set forcing, and store in global patches for access by the microcode

```
patches.fu = 10*exp(-patches.x.^2-patches.y.^2-patches.z.^2);
patches.fu = patches.fu.*(1+rand(size(patches.fu)));
```

Solve for steady state Set initial guess of zero, with `NaN` to indicate patch-edge values. Index `i` are the indices of patch-interior points, store in global patches for access by `theRes`, and the number of unknowns is then its number of elements.

```
u0 = zeros([nSubP,1,1,nPatch,nPatch,nPatch]);
u0([1 end],:,:,:) = nan;
u0(:,[1 end],:,:) = nan;
u0(:,:,[1 end],:) = nan;
patches.i = find(~isnan(u0));
nVariables = numel(patches.i)
```

Solve by iteration. Use `fsolve` for simplicity and robustness (optionally `optimoptions` to omit trace information), via the generic patch system wrapper `theRes` (Section 11).

```
disp('Solving system, takes 10--40 secs'),tic
uSoln = fsolve(@theRes,u0(patches.i) ...
        ,optimoptions('fsolve','Display','off'));
solveTime = toc
normResidual = norm(theRes(uSoln))
normSoln = norm(uSoln)
```

Store the solution into the patches, and give magnitudes.

```
u0(patches.i) = uSoln;
u0 = patchEdgeInt3(u0);
```

Plot isosurfaces of the solution

```
figure(1), clf
rgb=get(gca,'defaultAxesColorOrder');
```

Reshape spatial coordinates of patches.

```
x = patches.x(:);  y = patches.y(:);  z = patches.z(:);
```

Draw isosurfaces. Get the solution with interpolated faces, form into a 6D array, and reshape and transpose x and y to suit the isosurface function.

```
u = reshape( permute(squeeze(u0),[2 5 1 4 3 6]) ...
           , [numel(y) numel(x) numel(z)]);
maxu=max(u(:)),  minu=min(u(:))
```

Optionally cut-out the front corner so we can see inside.

```
  u( (x'>0) & (y<0) & (shiftdim(z,-2)>0) ) = nan;
```

Draw some isosurfaces.

```
clf;
for iso=5:-1:1
   isov=(iso-0.5)/5*(maxu-minu)+minu;
   hsurf(iso) = patch(isosurface(x,y,z,u,isov));
   isonormals(x,y,z,u,hsurf(iso))
   set(hsurf(iso) ,'FaceColor',rgb(iso,:) ...
       ,'EdgeColor','none' ,'FaceAlpha',iso/5);
   hold on
end
```

```
160 hold off
161 axis equal, axis([-1 1 -1 1 -1 1]), view(35,25)
162 xlabel('$x$'), ylabel('$y$'), zlabel('$z$')
163 camlight, lighting gouraud
164 ifOurCf2eps(mfilename) %optionally save plot
165 if exist('OurCf2eps') && OurCf2eps,  print('-dpng',['Figs/' mfilename
```

10.1 `microDiffBdry3()`: 3D forced heterogeneous diffusion with boundaries

This function codes the lattice forced heterogeneous diffusion inside the 3D patches. For 8D input array `u` (via edge-value interpolation of `patchEdgeInt3`, such as by `patchSys3`, **??**), computes the time derivative at each point in the interior of a patch, output in `ut`. The three 3D array of diffusivities, c^x_{ijk}, c^y_{ijk} and c^z_{ijk}, have previously been stored in `patches.cs` (4D).

Supply patch information as a third argument (required by parallel computation), or otherwise by a global variable.

```
191 function ut = microDiffBdry3(t,u,patches)
192   if nargin<3, global patches, end
```

Microscale space-steps.

```
198   dx = diff(patches.x(2:3));  % x micro-scale step
199   dy = diff(patches.y(2:3));  % y micro-scale step
200   dz = diff(patches.z(2:3));  % z micro-scale step
201   i = 2:size(u,1)-1; % x interior points in a patch
202   j = 2:size(u,2)-1; % y interior points in a patch
203   k = 2:size(u,3)-1; % y interior points in a patch
```

Code microscale boundary conditions of say Neumann on right, and Dirichlet on left, top, bottom, front, and back (viewed along the z-axis).

```
211   u( 1 ,:,:,:,:, 1 ,:,:)=0; %left face of leftmost patch
212   u(end,:,:,:,:,end,:,:)=u(end-1,:,:,:,:,end,:,:); %right face of rig
213   u(:, 1 ,:,:,:,:, 1 ,:)=0; %bottom face of bottommost
214   u(:,end,:,:,:,:,end,:)=0; %top face of topmost
215   u(:,:, 1 ,:,:,:,:, 1 )=0; %front face of frontmost
216   u(:,:,end,:,:,:,:,end)=0; %back face of backmost
```

Reserve storage and then assign interior patch values to the heterogeneous diffusion time derivatives. Using `nan+u` appears quicker than `nan(size(u),patches.codi`

```
  ut = nan+u; % reserve storage
  ut(i,j,k,:) ...
  = diff(patches.cs(:,j,k,1).*diff(u(:,j,k,:),1,1),1,1)/dx^2 ...
   +diff(patches.cs(i,:,k,2).*diff(u(i,:,k,:),1,2),1,2)/dy^2 ...
   +diff(patches.cs(i,j,:,3).*diff(u(i,j,:,:),1,3),1,3)/dz^2 ...
   +patches.fu(i,j,k);
end% function
```

11 theRes(): wrapper function to zero

This functions converts a vector of values into the interior values of the patches, then evaluates the time derivative of the system at time $t = 1$, and returns the vector of patch-interior time derivatives.

```
function f=theRes(u)
  global patches
  switch numel(size(patches.x))
    case 4, pSys = @patchSys1;
            v=nan(size(patches.x));
    case 5, pSys = @patchSys2;
            v=nan(size(patches.x+patches.y));
    case 6, pSys = @patchSys3;
            v=nan(size(patches.x+patches.y+patches.z));
    otherwise error('number of dimensions is somehow wrong')
  end%switch
  v(patches.i) = u;
  f = pSys(1,v(:),patches);
  f = f(patches.i);
end%function theRes
```

12 elastic2DstagHeteroSim: simulate 2D heterogeneous elastic patches on staggered grid

Execute patch scheme on the miscroscale grid of heterogeneous elasticity in a 2D beam as coded in the function `elastic2Dstaggered()` of Section 12.1. Here a beam of length π with either fixed or stress-free boundary conditions. This patch scheme provides an effective computational homogenisation of the microscale heterogeneous beam.

```
clear all
global patches
%global OurCf2eps, OurCf2eps=true %option to save plot
```

Set some patch and physical parameters

```
nPatch = 5
nSubP = 7
ny = 4
xLim = [0 pi]
yLim= [-1 1]*0.06
nVars = 4*ny-2;
iOrd = 0
edgyInt = true
heteroStrength = 1 % -2--2 ??
stressFreeRightBC = true
viscosity = 2e-3; % 1e-3 sometimes has unstable micro-modes!!!
tEnd = 30
basename = mfilename;
```

Viscosity of 1e-3 sometimes has unstable modes: only one pair for homogeneous beam, but three pairs for heterogeneous beam??

Set the cross-beam microscale y-coordinates and indices in row vectors: one for $u, \sigma_{xx}, \sigma_{yy}$-level; and one for v, σ_{xy}-level. Then show the micro-grid spacing.

```
yv=linspace(yLim(1),yLim(2),ny);
yu=(yv(1:ny-1)+yv(2:ny))/2;
ju=1:ny-1; jv=1:ny;
dy=diff(yu(1:2))
```

Physical elastic parameters—random Initially express in terms of Young's modulus and Poisson's ratio to be passed to the micro-code via `patches`. For heterogeneous elasticity, in the microgrid, we need λ at just nw-points, and μ at both nw,se points. Might as well provide at all quarter points as they both come from E, ν, so we need these two parameters at each of $2n_y - 1$ points across the beam. Edgy interpolation requires patches to be two microgrid points longer than any multiple of the microgrid periodicity, whereas non-edgy requires one more than an even multiple. Have to be careful with heterogeneities as nw,se-points are alternately either side of the notional microgrid lines.

```
xHeteroPeriod = (nSubP-1-edgyInt)/(2-edgyInt)
E  =  1*exp(heteroStrength*0.5*randn(xHeteroPeriod,2*ny-1)  );
nu = 0.3 +heteroStrength*0.1*(2*rand(xHeteroPeriod,2*ny-1)-1);
Equantiles  = quantile( E(:),[0:0.25:1])
nuQuantiles = quantile(nu(:),[0:0.25:1])
```

Compute corresponding λ, μ-fields, and store so `configPatches1` x-expands micro-heterogeneity to fill patch as necessary.

```
lambda=nu.*E./(1+nu)./(1-2*nu);
mu    =    E./(1+nu)./2;
cElas = [mu lambda];
```

Configure patches Using `hetCoeffs` to manage form heterogeneity in the patch, and adjoin viscosity coefficient.

```
Dom.type='equispace';
Dom.bcOffset = [ 0 0.75*stressFreeRightBC ];
configPatches1(@elastic2Dstaggered,xLim,'equispace',nPatch ...
    ,iOrd,dy,nSubP,'EdgyInt',edgyInt,'hetCoeffs',cElas);
patches.viscosity = viscosity;
patches.stressFreeRightBC = stressFreeRightBC;
dx=diff(patches.x(1:2))
```

Set initial condition Say choose initial velocities zero, and displacements varying somehow.

```
U0 = zeros(nSubP,nVars,1,nPatch);
U0(:,ju,:,:) = 0.1*sin(patches.x/(1+stressFreeRightBC))+0.*yu;
if stressFreeRightBC
     U0(:,jv+ju(end),:,:) = 0.02*patches.x.^2.*(2.5-patches.x)+0.*yv;
else U0(:,jv+ju(end),:,:) = 0.2*sin(patches.x)+0.*yv;
end
```

Optionally test the function

```
if 1 % test the new function
Ut=elastic2Dstaggered(-1,U0,patches);
Ut=reshape(Ut,nSubP,nVars,nPatch);
dudt=squeeze(Ut(:,ju,:))
dvdt=squeeze(Ut(:,jv+ju(end),:))
```

```
dutdt=squeeze(Ut(:,ju+2*ny-1,:))
dvtdt=squeeze(Ut(:,jv+2*ny-1+ju(end),:))
return
end
```

Integrate in time

```
[ts,Us] = ode15s(@patchSys1, [0 tEnd], U0(:));
```

Plot summary of simulation First, subsample the time-steps to roughly 150 steps.

```
nt=numel(ts)
jt=1:ceil(nt/150):nt;
ts=ts(jt);
Us=reshape(Us(jt,:),[],nSubP,nVars,1,nPatch);
```

Extract displacement fields.

```
us=Us(:,:,ju,:,:);
vs=Us(:,:,jv+ju(end),:,:);
```

Form arrays of averages and variation across y, reshaped into 2D arrays.

```
uMean=reshape(mean(us,3),[],nSubP*nPatch);
uStd=reshape(std(us,0,3),[],nSubP*nPatch);
vMean=reshape(mean(vs,3),[],nSubP*nPatch);
vStd=reshape(std(vs,0,3),[],nSubP*nPatch);
```

Plot xt-meshes coloured by the variation across y, first the u-field of compression waves, see **??**. The small space-shift in x-location is due to the staggered micro-grid for the patches as coded.

```
xs = patches.x;  xs([1 end],:) = nan;
figure(1),clf
mesh(xs(:)+dx/4,ts,uMean,uStd);
ylabel('time $t$'),xlabel('space $x$'),zlabel('mean $u$')
xlim([0 pi]),view(40,55),colorbar
ifOurCf2eps([basename 'us'])%optionally save
```

Draw the v-field showing the beam bending, see **??**. The small space-shift in x-location is due to the staggered micro-grid for the patches as coded.

```
figure(2),clf
mesh(xs(:)-dx/4,ts,vMean,vStd);
ylabel('time $t$'),xlabel('space $x$'),zlabel('mean $v$')
xlim([0 pi]),view(40,55),colorbar
drawnow
ifOurCf2eps([basename 'vs'])%optionally save
```

Compute Jacobian and its spectrum The aim here is four-fold:

- to show the patch scheme is stable for all elastic waves;
- to have a clear separation between fast and slow waves;
- for compression macro-waves to match theory of frequency $\omega = \sqrt{E}k$ for integer wavenumber k; and
- for beam macro-waves to match beam theory of $mv_{tt} = EIv_{xxxx}$ for mass-density $m := 2h$ and moment $I := \int_{-h}^{h} y^2\,dy = \frac{2}{3}h^3$ giving frequencies $\omega = \sqrt{E/3h}k$ where h is the half-width of the beam.

Form the Jacobian matrix, the linear operator, by numerical construction about a zero field. Use `i` to store the indices of the micro-grid points that are interior to the patches and hence are the system variables.

```
  u0 = zeros(nSubP,nVars,1,nPatch);
  u0([1 end],:,:,:)=nan; u0=u0(:);
  i=find(~isnan(u0));
  nVariables=length(i)
  Jac=nan(nVariables);
  for j=1:nVariables
    u0(i)=((1:nVariables)==j);
    dudt=patchSys1(0,u0);
    Jac(:,j)=dudt(i);
  end
  nJacEffZero = sum(abs(Jac(:))<1e-12)
  Jac(abs(Jac)<1e-12) = 0;
```

Find the eigenvalues of the Jacobian, and list the slowest for inspection.

```
  [evecs,evals]=eig(Jac);
  cabs=@(z) -real(z)*1e5+abs(imag(z));
  [~,j]=sort(cabs(diag(evals)));
```

```
  evals=diag(evals(j,j));  evecs=evecs(:,j);
  nZeroEvals=sum(abs(evals)<1e-5)
  j=find(abs(evals)>1e-5);
  leadingNonzeroEvals=evals(j(1:4*nPatch))
```

Plot quasi-log view of the spectrum, see **??**.

```
  figure(3),clf
  handle = plot(real(evals),imag(evals),'.');
  xlabel('real-part'), ylabel('imag-part')
  quasiLogAxes(handle,0.01,0.1);
  ifOurCf2eps([basename 'Eig'])%optionally save
```

12.1 `elastic2Dstaggered()`: $\partial/\partial t$ of 2D heterogeneous elastic patch on staggered grid

Let's try a staggered microgrid for patches of heterogeneous 2D elasticity forming a 2D beam. Figure 13 draw the microgrid in a patches: the microgrid is akin to that by Virieux (1986).

```
function [Ut]=elastic2Dstaggered(t,U,patches)
```

Input

- `t` is time (real scalar).
- `U` is vector of $(u, v, \dot{u}, \dot{v})$ values in each and every patch.
- `patches` data structure from `configPatches`, with extra physical parameters.

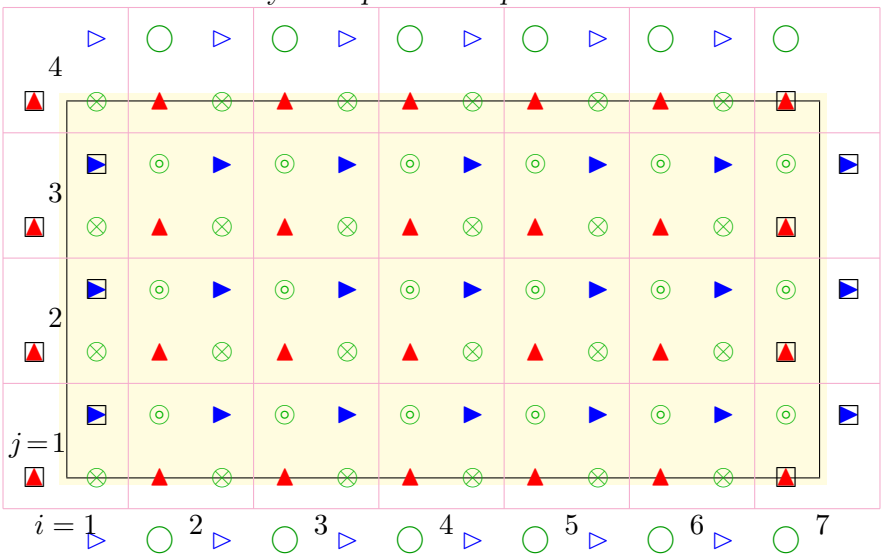
Output

- `Ut` is corresponding vector of time derivatives of `U`

Unpack the data vector Form data vector into a 4D array: `nx` is the number of points along a patch; `Nx` is the number of patches.

```
[nx,~,~,Nx] = size(patches.x);
nEnsem = patches.nEnsem;
nVars = round(numel(U)/numel(patches.x)/nEnsem);
U = reshape(U,nx,nVars,nEnsem,Nx);
```

Figure 13: microscale staggered xy-grid in a patch of the 2D beam (boxed pale yellow), the case of $n_{subpatch} = 7$ and $n_y = 4$: ▶, horizontal displacement u; ▲, vertical displacement v; ⊗, strains $\varepsilon_{yx} = \varepsilon_{xy}$ and stresses σ_{yx}, σ_{xy}; ◎, strains $\varepsilon_{yy}, \varepsilon_{xx}$ and stresses σ_{yy}, σ_{xx}. Open symbols represent values at ghost nodes outside the beam-patch determined by BCs. Symbols in squares are edge-values determined by inter-patch interpolation.



Set microgrid parameters of patches like Figure 13.

```
ny=(nVars+2)/4;
nny=2*ny-1;
dx=diff(patches.x(2:3));
dy=dx; % now set by new sim script
i =2:nx-1;  % indices for interior x
ix=1:nx-1;
ju=1:ny-1; % indices y structures of u, u_t
jv=1:ny;   % indices y structures of v, v_t
jse=1:2:nny; jnw=2:2:nny; % indices of elasticity y structure
```

Then split input field into the four physical fields.

```
u = U(:,ju        ,:,:);
v = U(:,jv+ju(end),:,:);
ut= U(:,ju+nny,:,:);
vt= U(:,jv+nny+ju(end),:,:);
```

Unpack the physical, microscale heterogeneous, elastic parameters.

```
mu  =patches.cs(:,1:nny);
lamb=patches.cs(:,2*ny:end);
visc=patches.viscosity;
```

Temporary trace print.

```
    if t<0
    usz=size(u),us=squeeze(u);
    vsz=size(v),vs=squeeze(v);
    utsz=size(ut),uts=squeeze(ut);
    vtsz=size(vt),vts=squeeze(vt);
    musz=size(mu),mus=squeeze(mu);
    lambsz=size(lamb),lambs=squeeze(lamb);
    end
```

Mathematical expression of elasticity Strain tensor $\varepsilon_{ij} := \frac{1}{2}(u_{i,j} + u_{j,i})$ is symmetric. Remember stress σ_{ij} is the force in the jth direction across a surface whose normal is the ith direction. So across a surface whose normal is $\vec{n}$, the stress is $\vec{n}^T\sigma$, equivalently $n_i\sigma_{ij}$.

Denote the 2D displacement vector by $\vec{u} = (u, v)$. [9] First, consider the x-direction. Substitute the strain-displacement equations into the equilibrium equation in the x-direction to get

$$\sigma_{xx} = 2\mu\varepsilon_{xx} + \lambda(\varepsilon_{xx} + \varepsilon_{yy}) = (2\mu + \lambda)\frac{\partial u}{\partial x} + \lambda\frac{\partial v}{\partial y}$$

$$\sigma_{xy} = 2\mu\varepsilon_{xy} = \mu\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right)$$

Discretise in space Form equi-spaced microscale grid of spacing dx, dy and indices i, j in the x, y-directions respectively (Figure 13). Field values are at various 'quarter points' within the microgrid elements (ne, nw, sw, se).

- locate u at ne-points
- locate v at sw-points
- evaluate diagonal strains $\varepsilon_{xx}, \varepsilon_{yy}$ at nw-points, also λ, μ

[9] Adapted from Wikipedia: linear elasticity: Derivation of Navier–Cauchy equations

- evaluate off-diagonal strains $\varepsilon_{xy} = \varepsilon_{yx}$ at se-points, also μ.
- evaluate PDEs at the appropriate sw,ne points, via gradients of stresses from the nw,se points.

All the above derivatives in space then involve simple first differences from grid points half-spacing away. They do *not* involve any averaging. Such staggered spatial discretisation is the best chance of best behaviour.

For interpolation between patches in the x-direction, that edge values of u, v are in zig-zag positions makes absolutely no difference to the patch interpolation schemes, since all coded schemes are invariant to translations in the x-direction just so long as the translation is the same across all patches for each of the edge variables.

Physical boundary conditions on extreme patches Fixed boundaries are to simply code zero displacements and zero time derivatives (velocities) at the boundaries. First at the left edge of the leftmost patch:

```
156 tweak=1;% choose simple zero, or accurate one??
157 u(1,:,:,1) =  +u(2,:,:,1)/5*tweak;
158 v(1,:,:,1) =  -v(2,:,:,1)/3*tweak;
159 ut(1,:,:,1)= +ut(2,:,:,1)/5*tweak;
160 vt(1,:,:,1)= -vt(2,:,:,1)/3*tweak;
```

Second, at the right edge of the rightmost patch: first alternative is fixed boundary.

```
167 if ~patches.stressFreeRightBC
168 u(nx,:,:,Nx) =  -u(nx-1,:,:,Nx)/3*tweak;
169 v(nx,:,:,Nx) =  +v(nx-1,:,:,Nx)/5*tweak;
170 ut(nx,:,:,Nx)= -ut(nx-1,:,:,Nx)/3*tweak;
171 vt(nx,:,:,Nx)= +vt(nx-1,:,:,Nx)/5*tweak;
```

otherwise code a stress free boundary at the location of the x-direction displacements and velocities (as for the top-bottom boundaries).

```
179 else% patches.stressFreeRightBC
```

Need `sxy` (below) to be computed zero at the bdry—assume u fattened by zero difference in y at top/bottom. Later set `sxx` to zero.

```
187 uDy = diff(u(nx-1,:,:,Nx),1,2);
188 v(nx,:,:,Nx) = v(nx-1,:,:,Nx)-dx/dy*[0 uDy 0];
```

For phenomenological viscosity purposes assume $\partial\dot{u}/\partial x = \partial\dot{v}/\partial x = 0$ at the free boundary.

```
vt(nx,:,:,Nx) = vt(nx-1,:,:,Nx);
ut(nx,:,:,Nx) = ut(nx-2,:,:,Nx);
end%if ~patches.stressFreeRightBC
```

Patch-interior elasticity For the case of Figure 13, fatten `u` using zero stress on top-bottom, although not really needed it does mean that σ_{xy} computed next is zero on the top-bottom.

```
u= [nan(nx,1,nEnsem,Nx)  u  nan(nx,1,nEnsem,Nx) ];
u(ix,1   ,:,:)=u(ix,2 ,:,:)+dy/dx*diff(v(:,1 ,:,:));
u(ix,ny+1,:,:)=u(ix,ny,:,:)-dy/dx*diff(v(:,ny,:,:));
```

- Compute stresses σ_{xy} at se-points.

```
sxy = mu(ix,jse).*( diff(u(ix,:,:,:),1,2)/dy+diff(v)/dx );
```

- Compute stresses σ_{yy} at nw-points (omitting leftmost σ_{yy}), fattening the array to cater for ghost nodes. Little tricky with indices of nw-elasticity parameters as they cross over the 'grid lines'.

```
syy = nan(nx,ny+1,nEnsem,Nx);
syy(ix+1,ju+1,:,:) =  ...
      (2*mu(:,jnw)+lamb(:,jnw)).*diff(v(ix+1,:,:,:),1,2)/dy ...
      +lamb(:,jnw).*diff(u(:,2:ny,:,:))/dx;
```

- Compute σ_{xx} at nw-points (omitting leftmost $i = 1$).

```
sxx = lamb(:,jnw).*diff(v(ix+1,:,:,:),1,2)/dy ...
     +(2*mu(:,jnw)+lamb(:,jnw)).*diff(u(:,ju+1,:,:))/dx;
```

Top-bottom boundary conditions At the top-bottom of the beam we need $\sigma_{xy} = \sigma_{yy} = 0$. Given the micro-grid of Figure 13, the first is already catered for. Here use $\sigma_{yy} = 0$ at sw points on the top-bottom to set ghost values.

```
syy(:,   1,:,:) = -syy(:,2 ,:,:);
syy(:,ny+1,:,:) = -syy(:,ny,:,:);
```

Similarly for any stress-free right boundary condition (remembering `sxx` currently omits leftmost $i = 1$).

```
if patches.stressFreeRightBC
  sxx(nx-1,:,:,Nx) = -sxx(nx-2,:,:,Nx);
end
```

Temporary trace print.

```
   if t<0
   sxysz=size(sxy),sxys=squeeze(sxy);
   syysz=size(syy),syys=squeeze(syy);
   sxxsz=size(sxx),sxxs=squeeze(sxx);
   end
```

Second derivatives for viscosity This code is for constant viscosity—if spatially varying, then modify each to be two first-derivatives in each direction. The x-derivatives are well-defined second differences.

```
utxx = visc*diff(ut,2,1)/dx^2;
vtxx = visc*diff(vt,2,1)/dx^2;
```

On Figure 13, and for the purpose of viscosity, assume $\partial\dot{u}/\partial y = \partial\dot{v}/\partial y = 0$ on the top-bottom (we just need 'viscosity' to be some phenomenological dissipation).

```
utyy = visc*diff(ut(i,[1 ju ny-1],:,:),2,2)/dy^2;
vtyy = visc*diff(vt(i,[2 jv ny-1],:,:),2,2)/dy^2;
```

Temporary trace print.

```
   if t<0
   utxxsz=size(utxx),utxxs=squeeze(utxx);
   vtxxsz=size(vtxx),vtxxs=squeeze(vtxx);
   utyysz=size(utyy),utyys=squeeze(utyy);
   vtyysz=size(vtyy),vtyys=squeeze(vtyy);
   end
```

Time derivatives The rate of change of displacement is the provided velocities: $\partial u/\partial t = \dot{u}$ and $\partial v/\partial t = \dot{v}$. Time derivative array should really be initialised to `nan`, but `ode15s` chokes on any `nan`s at the patch edges.

```
Ut=zeros(nx,nVars,nEnsem,Nx);
Ut(i,ju        ,:,:) = ut(i,:,:,:); % dudt = ut
Ut(i,jv+ju(end),:,:) = vt(i,:,:,:); % dvdt = vt
```

Substitute the stresses into the dynamical PDEs in the x-direction to get

$$\rho\frac{\partial \dot{u}}{\partial t} = \frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{yx}}{\partial y} + \kappa(\dot{u}_{xx} + \dot{u}_{yy}) + F_x\,,$$

and correspondingly for the y-direction. Here, we include some viscous dissipation of strength $\kappa =$ `visc`, but *do not* justify it as visco-elasticity. First code above x-direction, then the corresponding y-direction.

```
336 Ut(i,ju+nny,:,:) ...
337     = diff(sxx)/dx +diff(sxy(i,:,:,:),1,2)/dy +(utxx+utyy);
338 Ut(i,jv+nny+ju(end),:,:) ...
339     = diff(syy(i,:,:,:),1,2)/dy +diff(sxy)/dx +(vtxx+vtyy);
```

End of function.

New configuration and interpolation

13 `patchEdgeInt1()`: sets patch-edge values from interpolation over the 1D macroscale

Couples 1D patches across 1D space by computing their edge values from macroscale interpolation of either the mid-patch value (Roberts 2003; Roberts and Kevrekidis 2007), or the patch-core average (Bunder, Roberts, and Kevrekidis 2017), or the opposite next-to-edge values (Bunder, Kevrekidis, and Roberts 2021)—this last alternative often maintains symmetry. This function is primarily used by `patchSys1()` but is also useful for user graphics. When using core averages (not fully implemented), assumes the averages are sensible macroscale variables: then patch edge values are determined by macroscale interpolation of the core averages (Bunder, Roberts, and Kevrekidis 2017). [10]

Communicate patch-design variables via a second argument (optional, except required for parallel computing of `spmd`), or otherwise via the global struct `patches`.

```
31 function u=patchEdgeInt1(u,patches)
32 if nargin<2, global patches, end
```

[10] Script `patchEdgeInt1test.m` verifies this code.

Input

- `u` is a vector/array of length `nSubP` · `nVars` · `nEnsem` · `nPatch` where there are `nVars`·`nEnsem` field values at each of the points in the `nSubP` × `nPatch` multiscale spatial grid.
- `patches` a struct largely set by `configPatches1()`, and which includes the following.
  - `.x` is `nSubP` × 1 × 1 × `nPatch` array of the spatial locations x_{iI} of the microscale grid points in every patch. Currently it *must* be an equi-spaced lattice on the microscale index i, but may be variable spaced in macroscale index I.
  - `.ordCC` is order of interpolation, integer ≥ -1.
  - `.periodic` indicates whether macroscale is periodic domain, or alternatively that the macroscale has left and right boundaries so interpolation is via divided differences.
  - `.stag` in $\{0, 1\}$ is one for staggered grid (alternating) interpolation, and zero for ordinary grid.
  - `.Cwtsr` and `.Cwtsl` are the coupling coefficients for finite width interpolation—when invoking a periodic domain.
  - `.EdgyInt`, true/false, for determining patch-edge values by interpolation: true, from opposite-edge next-to-edge values (often preserves symmetry); false, from centre-patch values (original scheme).
  - `.nEnsem` the number of realisations in the ensemble.
  - `.parallel` whether serial or parallel.
  - `.nCore` [11]

Output

- `u` is 4D array, `nSubP` × `nVars` × `nEnsem` × `nPatch`, of the fields with edge values set by interpolation.

Test for reality of the field values, and define a function accordingly. Could be problematic if some variables are real and some are complex, or if variables are of quite different sizes.

[11] **ToDo:** introduced sometime but not fully implemented yet, because prefer ensemble

```
111   if max(abs(imag(u(:))))<1e-9*max(abs(u(:)))
112        uclean=@(u) real(u);
113   else uclean=@(u) u;
114   end
```

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

```
122 [nx,~,~,Nx] = size(patches.x);
123 nEnsem = patches.nEnsem;
124 nVars = round(numel(u)/numel(patches.x)/nEnsem);
125 assert(numel(u) == nx*nVars*nEnsem*Nx ...
126   ,'patchEdgeInt1: input u has wrong size for parameters')
127 u = reshape(u,nx,nVars,nEnsem,Nx);
```

If the user has not defined the patch core, then we assume it to be a single point in the middle of the patch, unless we are interpolating from next-to-edge values.

These index vectors point to patches and their two immediate neighbours, for periodic domain.

```
138 I = 1:Nx; Ip = mod(I,Nx)+1; Im = mod(I-2,Nx)+1;
```

Calculate centre of each patch and the surrounding core (`nx` and `nCore` are both odd).

```
145 i0 = round((nx+1)/2);
146 c = round((patches.nCore-1)/2);
```

13.1 Periodic macroscale interpolation schemes

```
155 if patches.periodic
```

Get the size ratios of the patches, then use finite width stencils or spectral.

```
162 r = patches.ratio(1);
163 if patches.ordCC>0 % then finite-width polynomial interpolation
```

Lagrange interpolation gives patch-edge values Consequently, compute centred differences of the patch core/edge averages/values for the macro-interpolation of all fields. Here the domain is macro-periodic.

```
173   if patches.EdgyInt % interpolate next-to-edge values
174     Ux = u([2 nx-1],:,:,I);
175   else % interpolate mid-patch values/sums
176     Ux = sum( u((i0-c):(i0+c),:,:,I) ,1);
177   end;
```

Just in case any last array dimension(s) are one, we have to force a padding of the sizes, then adjoin the extra dimension for the subsequent array of differences.

```
185 szUx0=size(Ux);
186 szUx0=[szUx0 ones(1,4-length(szUx0)) patches.ordCC];
```

Use finite difference formulas for the interpolation, so store finite differences in these arrays. When parallel, in order to preserve the distributed array structure we use an index at the end for the differences.

```
195   if patches.parallel
196     dmu = zeros(szUx0,patches.codist); % 5D
197   else
198     dmu = zeros(szUx0); % 5D
199   end
```

First compute differences, either μ and δ, or $\mu\delta$ and δ^2 in space.

```
206   if patches.stag % use only odd numbered neighbours
207     dmu(:,:,:,I,1) = (Ux(:,:,:,Ip)+Ux(:,:,:,Im))/2; % \mu
208     dmu(:,:,:,I,2) = (Ux(:,:,:,Ip)-Ux(:,:,:,Im)); % \delta
209     Ip = Ip(Ip); Im = Im(Im); % increase shifts to \pm2
210   else % standard
211     dmu(:,:,:,I,1) = (Ux(:,:,:,Ip)-Ux(:,:,:,Im))/2; % \mu\delta
212     dmu(:,:,:,I,2) = (Ux(:,:,:,Ip)-2*Ux(:,:,:,I) ...
213                       +Ux(:,:,:,Im)); % \delta^2
214   end%if patches.stag
```

Recursively take δ^2 of these to form successively higher order centred differences in space.

```
221   for k = 3:patches.ordCC
222     dmu(:,:,:,:,k) =       dmu(:,:,:,Ip,k-2) ...
223       -2*dmu(:,:,:,I,k-2) +dmu(:,:,:,Im,k-2);
224   end
```

Interpolate macro-values to be Dirichlet edge values for each patch (Roberts and Kevrekidis 2007; Bunder, Roberts, and Kevrekidis 2017), using weights computed in `configPatches1()`. Here interpolate to specified order.

For the case where single-point values interpolate to patch-edge values: when we have an ensemble of configurations, different realisations are coupled to each other as specified by `patches.le` and `patches.ri`.

```
  if patches.nCore==1
    k=1+patches.EdgyInt; % use centre/core or two edges
    u(nx,:,patches.ri,I) = Ux(1,:,:,:)*(1-patches.stag) ...
      +sum( shiftdim(patches.Cwtsr,-4).*dmu(1,:,:,:,:) ,5);
    u(1 ,:,patches.le,I) = Ux(k,:,:,:)*(1-patches.stag) ...
      +sum( shiftdim(patches.Cwtsl,-4).*dmu(k,:,:,:,:) ,5);
```

For a non-trivial core then more needs doing: the core (one or more) of each patch interpolates to the edge action regions. When more than one in the core, the edge is set depending upon near edge values so the average near the edge is correct.

```
  else% patches.nCore>1
    error('not yet considered, july--dec 2020 ??')
    u(nx,:,:,I) = Ux(:,:,I)*(1-patches.stag) ...
      + reshape(-sum(u((nx-patches.nCore+1):(nx-1),:,:,I),1) ...
      + sum( patches.Cwtsr.*dmu ),Nx,nVars);
    u(1,:,:,I) = Ux(:,:,I)*(1-patches.stag) ...
      + reshape(-sum(u(2:patches.nCore,:,:,I),1)  ...
      + sum( patches.Cwtsl.*dmu ),Nx,nVars);
  end%if patches.nCore
```

Case of spectral interpolation Assumes the domain is macro-periodic.

```
else% patches.ordCC<=0, spectral interpolation
```

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 `Nx` patches we resolve 'wavenumbers' $|k| < \texttt{Nx}/2$, so set row vector $\texttt{ks} = k2\pi/N$ for 'wavenumbers' $k = (0\,,1\,,\ldots,k_{\max}\,,-k_{\max}\,,\ldots,-1)$ for odd N, and $k = (0\,,1\,,\ldots,k_{\max}\,,(k_{\max}+1)\,,-k_{\max}\,,\ldots,-1)$ for even N.

Deal with staggered grid by doubling the number of fields and halving the number of patches (`configPatches1()` tests that 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. [12]

```
  if patches.stag % transform by doubling the number of fields
    v = nan(size(u)); % currently to restore the shape of u
    u = [u(:,:,:,1:2:Nx) u(:,:,:,2:2:Nx)];
    stagShift = 0.5*[ones(1,nVars) -ones(1,nVars)];
    iV = [nVars+1:2*nVars 1:nVars]; % scatter interp to alternate fie
    r = r/2;           % ratio effectively halved
    Nx = Nx/2; % halve the number of patches
    nVars = nVars*2;   % double the number of fields
  else % the values for standard spectral
    stagShift = 0;
    iV = 1:nVars;
  end%if patches.stag
```

Now set wavenumbers (when `Nx` is even then highest wavenumber is π).

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

Compute the Fourier transform across patches of the patch centre or next-to-edge values for all the fields. If there are an even number of points, then if complex, treat as positive wavenumber, but if real, treat as cosine. When using an ensemble of configurations, different configurations might be coupled to each other, as specified by `patches.le` and `patches.ri`.

```
if ~patches.EdgyInt
    Cleft = fft(u(i0  ,:,:,:),[],4);
    Cright = Cleft;
else
    Cleft = fft(u(2   ,:,:,:),[],4);
    Cright= fft(u(nx-1,:,:,:),[],4);
end
```

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

[12] **ToDo:** Have not yet tested whether works for Edgy Interpolation.

```
343   u(nx,iV,patches.ri,:) = uclean( ifft( ...
344       Cleft.*exp(1i*ks.*(stagShift+r)) ,[],4));
345   u(1 ,iV,patches.le,:) = uclean( ifft( ...
346       Cright.*exp(1i*ks.*(stagShift-r)) ,[],4));
```

Restore staggered grid when appropriate. This dimensional shifting appears to work. Is there a better way to do this?

```
354 if patches.stag
355   nVars = nVars/2;
356   u=reshape(u,nx,nVars,2,nEnsem,Nx);
357   Nx = 2*Nx;
358   v(:,:,:,1:2:Nx) = u(:,:,1,:,:);
359   v(:,:,:,2:2:Nx) = u(:,:,2,:,:);
360   u = v;
361 end%if patches.stag
362 end%if patches.ordCC
```

13.2 Non-periodic macroscale interpolation

```
370 else% patches.periodic false
371 assert(~patches.stag, ...
372 'not yet implemented staggered grids for non-periodic')
```

Determine the order of interpolation `p`, and hence size of the (forward) divided difference table in `F`.

```
379 if patches.ordCC<1, patches.ordCC = Nx-1; end
380 p = min(patches.ordCC,Nx-1);
381 F = nan(patches.EdgyInt+1,nVars,nEnsem,Nx,p+1);
```

Set function values in first 'column' of the table for every variable and across ensemble. For `EdgyInt`, the 'reversal' of the next-to-edge values are because their values are to interpolate to the opposite edge of each patch.

```
391   if patches.EdgyInt % interpolate next-to-edge values
392     F(:,:,:,:,1) = u([nx-1 2],:,:,I);
393     X(:,:,:,:) = patches.x([nx-1 2],:,:,I);
394   else % interpolate mid-patch values/sums
395     F(:,:,:,:,1) = sum( u((i0-c):(i0+c),:,:,I) ,1);
396     X(:,:,:,:) = patches.x(i0,:,:,I);
397   end;
```

Compute table of (forward) divided differences (e.g., Wikipedia 2022) for every variable and across ensemble.

```
for q = 1:p
  i = 1:Nx-q;
  F(:,:,:,i,q+1) = (F(:,:,:,i+1,q)-F(:,:,:,i,q)) ...
                  ./(X(:,:,:,i+q)  -X(:,:,:,i));
end
```

Now interpolate to the edge-values at locations `Xedge`.

```
Xedge = patches.x([1 nx],:,:,:);
```

Code Horner's evaluation of the interpolation polynomials. Indices `i` are those of the left end of each interpolation stencil because the table is of forward differences.[13] First alternative: the case of order p interpolation across the domain, asymmetric near the boundary. Use this first alternative for now.

```
if true
  i = max(1,min(1:Nx,Nx-ceil(p/2))-floor(p/2));
  Uedge = F(:,:,:,i,p+1);
  for q = p:-1:1
    Uedge = F(:,:,:,i,q)+(Xedge-X(:,:,:,i+q-1)).*Uedge;
  end
```

Second alternative: lower the degree of interpolation near the boundary to maintain the band-width of the interpolation. Such symmetry might be essential for multi-D. [14]

```
else%if false
  i = max(1,I-floor(p/2));
```

For the tapering order of interpolation, form the interior mask `Q` (logical) that signifies which interpolations are to be done at order `q`. This logical mask spreads by two as each order `q` decreases.

```
  Q = (I-1>=floor(p/2)) & (Nx-I>=p/2);
  Imid = floor(Nx/2);
```

[13] For EdgyInt, perhaps interpret odd order interpolation in such a way that first-order interpolations reduces to appropriate linear interpolation so that as patches abut the scheme is 'full-domain'. May mean left-edge and right-edge have different indices. Explore sometime??

[14] The aim is to preserve symmetry?? Does it?? As of Jan 2023 it only partially does—fails near boundaries, and maybe fails with uneven spacing.

Initialise to highest divide difference, surrounded by zeros.

```
464   Uedge = zeros(patches.EdgyInt+1,nVars,nEnsem,Nx);
465   Uedge(:,:,:,Q) = F(:,:,:,i(Q),p+1);
```

Complete Horner evaluation of the relevant polynomials.

```
471   for q = p:-1:1
472     Q = [Q(2:Imid) true(1,2) Q(Imid+1:end-1)]; % spread mask
473     Uedge(:,:,:,Q) = F(:,:,:,i(Q),q) ...
474         +(Xedge(:,:,:,Q)-X(:,:,:,i(Q)+q-1)).*Uedge(:,:,:,Q);
475   end%for q
476 end%if
```

Finally, insert edge values into the array of field values, using the required ensemble shifts.

```
484 u(1 ,:,patches.le,I) = Uedge(1,:,:,I);
485 u(nx,:,patches.ri,I) = Uedge(2,:,:,I);
```

We want a user to set the extreme patch edge values according to the microscale boundary conditions that hold at the extremes of the domain. Consequently, may override their computed interpolation values with `NaN`.

```
494 u( 1,:,:, 1) = nan;
495 u(nx,:,:,Nx) = nan;
```

End of the non-periodic interpolation code.

```
501 end%if patches.periodic
```

Fin, returning the 4D array of field values.

14 `configPatches1()`: configures spatial patches in 1D

Makes the struct `patches` for use by the patch/gap-tooth time derivative/step function `patchSys1()`. Section 14.1 lists an example of its use.

```
19 function patches = configPatches1(fun,Xlim,Dom ...
20     ,nPatch,ordCC,dx,nSubP,varargin)
```

Input If invoked with no input arguments, then executes an example of simulating Burgers' PDE—see Section 14.1 for the example code.

- `fun` is the name of the user function, `fun(t,u,patches)` or `fun(t,u)`, that computes time derivatives (or time-steps) of quantities on the 1D micro-grid within all the 1D patches.

- `Xlim` give the macro-space spatial domain of the computation, namely the interval [`Xlim(1)`, `Xlim(2)`].

- `Dom` sets the type of macroscale conditions for the patches, and reflects the type of microscale boundary conditions of the problem. If `Dom` is `NaN` or `[]`, then the field `u` is macro-periodic in the 1D spatial domain, and resolved on equi-spaced patches. If `Dom` is a character string, then that specifies the `.type` of the following structure, with `.bcOffset` set to the default zero. Otherwise `Dom` is a structure with the following components.

  - `.type`, string, of either `'periodic'` (the default), `'equispace'`, `'chebyshev'`, `'usergiven'`. For all cases except `'periodic'`, users *must* code into `fun` the micro-grid boundary conditions that apply at the left(right) edge of the leftmost(rightmost) patches.
  - `.bcOffset`, optional one or two element array, in the cases of `'equispace'` or `'chebyshev'` the patches are placed so the left/right macroscale boundaries are aligned to the left/right edges of the corresponding extreme patches, but offset by `bcOffset` of the sub-patch micro-grid spacing. For example, use `bcOffset=0` when applying Dirichlet boundary values on the extreme edge micro-grid points, whereas use `bcOffset=0.5` when applying Neumann boundary conditions halfway between the extreme edge micro-grid points.
  - `.X`, optional array, in the case `'usergiven'` it specifies the locations of the centres of the `nPatch` patches—the user is responsible it makes sense.

- `nPatch` is the number of equi-spaced spatial patches.

- `ordCC`, must be ≥ -1, is the 'order' of interpolation across empty space of the macroscale patch values to the edge of the patches for inter-patch coupling: where `ordCC` of 0 or -1 gives spectral interpolation; and `ordCC` being odd specifies staggered spatial grids.

- `dx` (real) is usually the sub-patch micro-grid spacing in x.

  However, if `Dom` is `NaN` (as for pre-2023), then `dx` actually is `ratio`, namely the ratio of (depending upon `EdgyInt`) either the half-width or full-width of a patch to the equi-spacing of the patch mid-points. So either `ratio` $= \frac{1}{2}$ means the patches abut and `ratio` $= 1$ is overlapping patches as in holistic discretisation, or `ratio` $= 1$ means the patches abut. Small `ratio` should greatly reduce computational time.

- `nSubP` is the number of equi-spaced microscale lattice points in each patch. If not using `EdgyInt`, then must be odd so that there is a centre-patch lattice point.

- `nEdge` (not yet implemented), *optional*, default=1, for each patch, the number of edge values set by interpolation at the edge regions of each patch. The default is one (suitable for microscale lattices with only nearest neighbour interactions).

- `EdgyInt`, true/false, *optional*, default=false. If true, then interpolate to left/right edge-values from right/left next-to-edge values. If false or omitted, then interpolate from centre-patch values.

- `nEnsem`, *optional-experimental*, default one, but if more, then an ensemble over this number of realisations.

- `hetCoeffs`, *optional*, default empty. Supply a 1D or 2D array of microscale heterogeneous coefficients to be used by the given microscale `fun` in each patch. Say the given array `cs` is of size $m_x \times n_c$, where n_c is the number of different sets of coefficients. The coefficients are to be the same for each and every patch; however, macroscale variations are catered for by the n_c coefficients being n_c parameters in some macroscale formula.

  - If `nEnsem` $= 1$, then the array of coefficients is just tiled across the patch size to fill up each patch, starting from the first point in each patch.
  - If `nEnsem` > 1 (value immaterial), then reset `nEnsem` $:= m_x$ and construct an ensemble of all m_x phase-shifts of the coefficients. In this scenario, the inter-patch coupling couples different members in the ensemble. When `EdgyInt` is true, and when the coefficients are diffusivities/elasticities, then this coupling cunningly preserves symmetry.

- `nCore`, *optional-experimental*, default one, but if more, and only for non-EdgyInt, then interpolates from an average over the core of a patch, a core of size ??. Then edge values are set according to interpolation of the averages?? or so that average at edges is the interpolant??

- `'parallel'`, true/false, *optional*, default=false. If false, then all patch computations are on the user's main CPU—although a user may well separately invoke, say, a GPU to accelerate sub-patch computations.

  If true, and it requires that you have MATLAB's Parallel Computing Toolbox, then it will distribute the patches over multiple CPUs/cores. In MATLAB, only one array dimension can be split in the distribution, so it chooses the one space dimension x. A user may correspondingly distribute arrays with property `patches.codist`, or simply use formulas invoking the preset distributed arrays `patches.x`. If a user has not yet established a parallel pool, then a 'local' pool is started.

Output The struct `patches` is created and set with the following components. If no output variable is provided for `patches`, then make the struct available as a global variable.[15]

```
180 if nargout==0, global patches, end
```

- `.fun` is the name of the user's function `fun(t,u,patches)` or `fun(t,u)`, that computes the time derivatives (or steps) on the patchy lattice.

- `.ordCC` is the specified order of inter-patch coupling.

- `.periodic`: either true, for interpolation on the macro-periodic domain; or false, for general interpolation by divided differences over non-periodic domain or unevenly distributed patches.

- `.stag` is true for interpolation using only odd neighbouring patches as for staggered grids, and false for the usual case of all neighbour coupling.

- `.Cwtsr` and `.Cwtsl`, only for macro-periodic conditions, are the `ordCC`-vector of weights for the inter-patch interpolation onto the right and left edges (respectively) with patch:macroscale ratio as specified or as derived from `dx`.

[15] When using `spmd` parallel computing, it is generally best to avoid global variables, and so instead prefer using an explicit output variable.

- `.x` (4D) is `nSubP` $\times 1 \times 1 \times$ `nPatch` array of the regular spatial locations x_{iI} of the ith microscale grid point in the Ith patch.
- `.ratio`, only for macro-periodic conditions, is the size ratio of every patch.
- `.nEdge` is, for each patch, the number of edge values set by interpolation at the edge regions of each patch.
- `.le`, `.ri` determine inter-patch coupling of members in an ensemble. Each a column vector of length `nEnsem`.
- `.cs` either
  - `[]` 0D, or
  - if `nEnsem` $= 1$, (`nSubP(1)` $- 1) \times n_c$ 2D array of microscale heterogeneous coefficients, or
  - if `nEnsem` > 1, (`nSubP(1)` $- 1) \times n_c \times m_x$ 3D array of m_x ensemble of phase-shifts of the microscale heterogeneous coefficients.
- `.parallel`, logical: true if patches are distributed over multiple CPUs/ cores for the Parallel Computing Toolbox, otherwise false (the default is to activate the *local* pool).
- `.codist`, *optional*, describes the particular parallel distribution of arrays over the active parallel pool.

14.1 If no arguments, then execute an example

```
252 if nargin==0
253 disp('With no arguments, simulate example of Burgers PDE')
```

The code here shows one way to get started: a user's script may have the following three steps (" $\mapsto$ " denotes function recursion).

1. configPatches1
2. ode15s integrator $\mapsto$ patchSys1 $\mapsto$ user's PDE
3. process results

Establish global patch data struct to point to and interface with a function coding Burgers' PDE: to be solved on 2π-periodic domain, with eight patches, spectral interpolation couples the patches, with micro-grid spacing 0.06, and with seven microscale points forming each patch.

```
global patches
patches = configPatches1(@BurgersPDE,[0 2*pi], [], 8, 0, 0.06, 7);
```

Set some initial condition, with some microscale randomness.

```
u0=0.3*(1+sin(patches.x))+0.1*randn(size(patches.x));
```

Simulate in time using a standard stiff integrator and the interface function `patchSys1()` (??).

```
if ~exist('OCTAVE_VERSION','builtin')
[ts,us] = ode15s( @patchSys1,[0 0.5],u0(:));
else % octave version
[ts,us] = odeOcts(@patchSys1,[0 0.5],u0(:));
end
```

Plot the simulation using only the microscale values interior to the patches: either set x-edges to `nan` to leave the gaps; or use `patchEdgyInt1` to re-interpolate correct patch edge values and thereby join the patches. Figure 14 illustrates an example simulation in time generated by the patch scheme applied to Burgers' PDE.

```
figure(1),clf
if 1, patches.x([1 end],:,:,:)=nan;  us=us.';
else us=reshape(patchEdgyInt1(us.'),[],length(ts));
end
surf(ts,patches.x(:),us)
view(60,40), colormap(0.8*hsv)
title('Burgers PDE: patches in space, continuous time')
xlabel('time t'), ylabel('space x'), zlabel('u(x,t)')
```

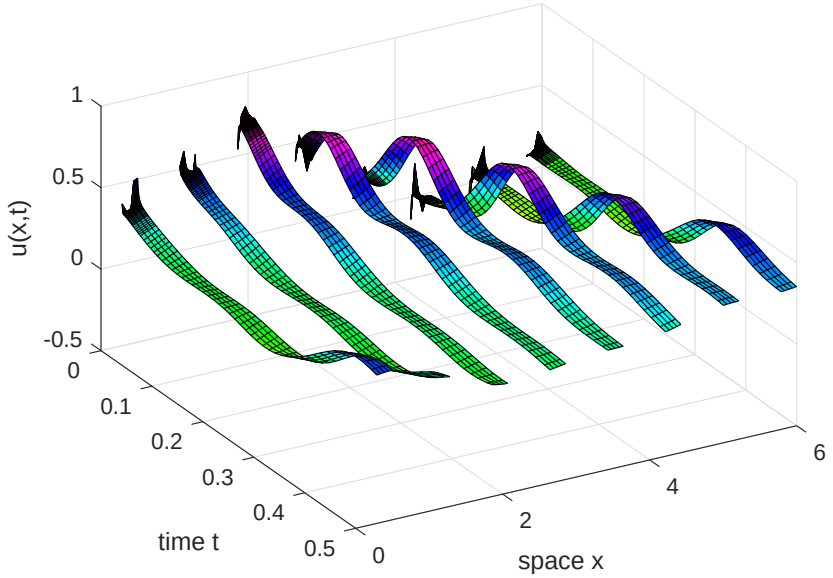
Upon finishing execution of the example, optionally save the graph to be shown in Figure 14, then exit this function.

```
ifOurCf2eps(mfilename)
return
end%if nargin==0
```

14.2 Parse input arguments and defaults

```
p = inputParser;
fnValidation = @(f) isa(f, 'function_handle'); %test for fn name
```

Figure 14: field $u(x,t)$ of the patch scheme applied to Burgers' PDE.




```
addRequired(p,'fun',fnValidation);
addRequired(p,'Xlim',@isnumeric);
%addRequired(p,'Dom'); % nothing yet decided
addRequired(p,'nPatch',@isnumeric);
addRequired(p,'ordCC',@isnumeric);
addRequired(p,'dx',@isnumeric);
addRequired(p,'nSubP',@isnumeric);
addParameter(p,'nEdge',1,@isnumeric);
addParameter(p,'EdgyInt',false,@islogical);
addParameter(p,'nEnsem',1,@isnumeric);
addParameter(p,'hetCoeffs',[],@isnumeric);
addParameter(p,'parallel',false,@islogical);
addParameter(p,'nCore',1,@isnumeric);
parse(p,fun,Xlim,nPatch,ordCC,dx,nSubP,varargin{:});
```

Set the optional parameters.

```
patches.nEdge = p.Results.nEdge;
patches.EdgyInt = p.Results.EdgyInt;
patches.nEnsem = p.Results.nEnsem;
```

```
cs = p.Results.hetCoeffs;
patches.parallel = p.Results.parallel;
patches.nCore = p.Results.nCore;
```

Check parameters.

```
assert(Xlim(1)<Xlim(2) ...
      ,'two entries of Xlim must be ordered increasing')
assert(patches.nEdge==1 ...
      ,'multi-edge-value interp not yet implemented')
assert(2*patches.nEdge+1<=nSubP ...
      ,'too many edge values requested')
if patches.nCore>1
    warning('nCore>1 not yet tested in this version')
    end
```

For compatibility with pre-2023 functions, if parameter `Dom` is `Nan`, then we set the `ratio` to be the value of the so-called `dx` parameter.

```
if ~isstruct(Dom), pre2023=isnan(Dom);
else pre2023=false; end
if pre2023, ratio=dx; dx=nan; end
```

Default macroscale conditions are periodic with evenly spaced patches.

```
if isempty(Dom), Dom=struct('type','periodic'); end
if (~isstruct(Dom))&isnan(Dom), Dom=struct('type','periodic'); end
```

If `Dom` is a string, then just set type to that string, and then get corresponding defaults for others fields.

```
if ischar(Dom), Dom=struct('type',Dom); end
```

Check what is and is not specified, and provide default of Dirichlet boundaries if no `bcOffset` specified when needed.

```
patches.periodic=false;
switch Dom.type
case 'periodic'
    patches.periodic=true;
    if isfield(Dom,'bcOffset')
    warning('bcOffset not available for Dom.type = periodic'), end
    if isfield(Dom,'X')
```

```
427     warning('X not available for Dom.type = periodic'), end
428 case {'equispace','chebyshev'}
429     if ~isfield(Dom,'bcOffset'), Dom.bcOffset=[0;0]; end
430     if length(Dom.bcOffset)==1
431         Dom.bcOffset=repmat(Dom.bcOffset,2,1); end
432     if isfield(Dom,'X')
433     warning('X not available for Dom.type = equispace or chebyshev')
434     end
435 case 'usergiven'
436     if isfield(Dom,'bcOffset')
437     warning('bcOffset not available for usergiven Dom.type'), end
438     assert(isfield(Dom,'X'),'X required for Dom.type = usergiven')
439 otherwise
440     error([Dom.type 'is unknown Dom.type'])
441 end%switch Dom.type
```

14.3 The code to make patches and interpolation

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

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

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

```
462 assert((ordCC>=-1) & (floor(ordCC)==ordCC), ...
463     'ordCC out of allowed range integer>=-1')
```

For odd `ordCC`, interpolate based upon odd neighbouring patches as is useful for staggered grids.

```
470 patches.stag=mod(ordCC,2);
471 ordCC=ordCC+patches.stag;
472 patches.ordCC=ordCC;
```

Check for staggered grid and periodic case.

```
478   if patches.stag, assert(mod(nPatch,2)==0, ...
479     'Require an even number of patches for staggered grid')
480   end
```

Third, set the centre of the patches in the macroscale grid of patches, depending upon `Dom.type`.

```
switch Dom.type
```

The periodic case is evenly spaced within the spatial domain. Store the size ratio in `patches`.

```
case 'periodic'
  X=linspace(Xlim(1),Xlim(2),nPatch+1);
  DX=X(2)-X(1);
  X=X(1:nPatch)+diff(X)/2;
  pEI=patches.EdgyInt;% abbreviation
  if pre2023, dx = ratio*DX/(nSubP-1-pEI)*(2-pEI);
  else        ratio = dx/DX*(nSubP-1-pEI)/(2-pEI);  end
  patches.ratio=ratio;
```

In the case of macro-periodicity, precompute the weightings to interpolate field values for coupling. [16]

```
  if ordCC>0
    [Cwtsr,Cwtsl] = patchCwts(ratio,ordCC,patches.stag);
    patches.Cwtsr = Cwtsr;  patches.Cwtsl = Cwtsl;
  end
```

The equi-spaced case is also evenly spaced but with the extreme edges aligned with the spatial domain boundaries, modified by the offset.

```
case 'equispace'
  X=linspace(Xlim(1)+((nSubP-1)/2-Dom.bcOffset(1))*dx ...
            ,Xlim(2)-((nSubP-1)/2-Dom.bcOffset(2))*dx ,nPatch);
  DX=diff(X(1:2));
  width=(1+patches.EdgyInt)/2*(nSubP-1-patches.EdgyInt)*dx;
  if DX<width*0.999999
     warning('too many equispace patches (double overlapping)')
     end
```

The Chebyshev case is spaced according to the Chebyshev distribution in order to reduce macro-interpolation errors, $X_i \propto -\cos(i\pi/N)$, but with the extreme edges aligned with the spatial domain boundaries, modified by the offset, and modified by possible 'boundary layers'.[17]

[16] **ToDo:** Might sometime extend to coupling via derivative values.

[17] However, maybe overlapping patches near a boundary should be viewed as some sort of spatial analogue of the 'christmas tree' of projective integration and its projection to a slow manifold. Here maybe the overlapping patches allow for a 'christmas tree' approach to the boundary layers. Needs to be explored??

```
548 case 'chebyshev'
549   halfWidth=dx*(nSubP-1)/2;
550   X1 = Xlim(1)+halfWidth-Dom.bcOffset(1)*dx;
551   X2 = Xlim(2)-halfWidth+Dom.bcOffset(2)*dx;
552 %  X = (X1+X2)/2-(X2-X1)/2*cos(linspace(0,pi,nPatch));
```

Search for total width of 'boundary layers' so that in the interior the patches are non-overlapping Chebyshev. But the width for assessing overlap of patches is the following variable `width`.

```
561   width=(1+patches.EdgyInt)/2*(nSubP-1-patches.EdgyInt)*dx;
562   for b=0:2:nPatch-2
563     DXmin=(X2-X1-b*width)/2*( 1-cos(pi/(nPatch-b-1)) );
564     if DXmin>width, break, end
565   end
566   if DXmin<width*0.999999
567      warning('too many Chebyshev patches (mid-domain overlap)')
568      end
```

Assign the centre-patch coordinates.

```
574   X = [ X1+(0:b/2-1)*width ...
575         (X1+X2)/2-(X2-X1-b*width)/2*cos(linspace(0,pi,nPatch-b)) ...
576         X2+(1-b/2:0)*width ];
```

The user-given case is entirely up to a user to specify, we just force it to have the correct shape of a row.

```
585 case 'usergiven'
586   X = reshape(Dom.X,1,[]);
587 end%switch Dom.type
```

Fourth, construct the microscale grid in each patch. Reshape the grid to be 4D to suit dimensions (micro,Vars,Ens,macro).

```
597 assert(patches.EdgyInt | mod(nSubP,2)==1, ...
598     'configPatches1: nSubP must be odd')
599 i0=(nSubP+1)/2;
600 patches.x = reshape( dx*(-i0+1:i0-1)'+X ,nSubP,1,1,nPatch);
```

14.4 Set ensemble inter-patch communication

For `EdgyInt` or centre interpolation respectively,

- the right-edge/centre realisations `1:nEnsem` are to interpolate to left-edge `le`, and
- the left-edge/centre realisations `1:nEnsem` are to interpolate to `re`.

`re` and `li` are 'transposes' of each other as `re(li)=le(ri)` are both `1:nEnsem`. Alternatively, one may use the statement

```
c=hankel(c(1:nSubP-1),c([nSubP 1:nSubP-2]));
```

to *correspondingly* generates all phase shifted copies of microscale heterogeneity (see `homoDiffEdgy1` of **??**).

The default is nothing shifty. This setting reduces the number of if-statements in function `patchEdgeInt1()`.

```
630 nE = patches.nEnsem;
631 patches.le = 1:nE;
632 patches.ri = 1:nE;
```

However, if heterogeneous coefficients are supplied via `hetCoeffs`, then do some non-trivial replications. First, get microscale periods, patch size, and replicate many times in order to subsequently sub-sample: `nSubP` times should be enough. If `cs` is more then 2D, then the higher-dimensions are reshaped into the 2nd dimension.

```
644 if ~isempty(cs)
645   [mx,nc] = size(cs);
646   nx = nSubP(1);
647   cs = repmat(cs,nSubP,1);
```

If only one member of the ensemble is required, then sub-sample to patch size, and store coefficients in `patches` as is.

```
655   if nE==1, patches.cs = cs(1:nx-1,:); else
```

But for `nEnsem` > 1 an ensemble of m_x phase-shifts of the coefficients is constructed from the over-supply. Here code phase-shifts over the periods—the phase shifts are like Hankel-matrices.

```
664     patches.nEnsem = mx;
665     patches.cs = nan(nx-1,nc,mx);
```

```
    for i = 1:mx
        is = (i:i+nx-2);
        patches.cs(:,:,i) = cs(is,:);
    end
    patches.cs = reshape(patches.cs,nx-1,nc,[]);
```

Further, set a cunning left/right realisation of inter-patch coupling. The aim is to preserve symmetry in the system when also invoking `EdgyInt`. What this coupling does without `EdgyInt` is unknown. Use auto-replication.

```
    patches.le = mod((0:mx-1)'+mod(nx-2,mx),mx)+1;
    patches.ri = mod((0:mx-1)'-mod(nx-2,mx),mx)+1;
```

Issue warning if the ensemble is likely to be affected by lack of scale separation. Need to justify this and the arbitrary threshold more carefully??

```
if ratio*patches.nEnsem>0.9, warning( ...
'Probably poor scale separation in ensemble of coupled phase-shifts')
scaleSeparationParameter = ratio*patches.nEnsem
end
```

End the two if-statements.

```
  end%if-else nEnsem>1
end%if not-empty(cs)
```

If parallel code then first assume this is not within an `spmd`-environment, and so we invoke `spmd...end` (which starts a parallel pool if not already started). At this point, the global `patches` is copied for each worker processor and so it becomes *composite* when we distribute any one of the fields. Hereafter, *all fields in the global variable* `patches` *must only be referenced within an* `spmd`*-environment.*[18]

```
if patches.parallel
%  theparpool=gcp()
  spmd
```

Second, choose to slice parallel workers in the spatial direction.

```
  pari = 1;
  patches.codist=codistributor1d(3+pari);
```

[18] If subsequently outside spmd, then one must use functions like `getfield(patches{1},'a')`.

patches.codist.Dimension is the index that is split among workers. Then distribute the coordinate direction among the workers: the function must be invoked inside an spmd-group in order for this to work—so we do not need parallel in argument list.

```
  switch pari
    case 1, patches.x=codistributed(patches.x,patches.codist);
  otherwise
    error('should never have bad index for parallel distribution')
  end%switch
  end%spmd
```

If not parallel, then clean out patches.codist if it exists. May not need, but safer.

```
else% not parallel
  if isfield(patches,'codist'), rmfield(patches,'codist'); end
end%if-parallel
```

Fin

```
end% function
```

15 patchEdgeInt2(): sets 2D patch edge values from 2D macroscale interpolation

Couples 2D patches across 2D space by computing their edge values via macroscale interpolation. Research (Roberts, MacKenzie, and Bunder 2014; Bunder et al. 2021) indicates the patch centre-values are sensible macroscale variables, and macroscale interpolation of these determine patch-edge values. However, for computational homogenisation in multi-D, interpolating patch next-to-edge values appears better (Bunder, Kevrekidis, and Roberts 2021). This function is primarily used by patchSys2() but is also useful for user graphics. [19]

Communicate patch-design variables via a second argument (optional, except required for parallel computing of spmd), or otherwise via the global struct patches.

```
function u = patchEdgeInt2(u,patches)
if nargin<2, global patches, end
```

[19] Script patchEdgeInt2test.m verifies this code.

Input

- `u` is a vector/array of length `prod(nSubP)·nVars·nEnsem·prod(nPatch)` where there are `nVars · nEnsem` field values at each of the points in the `nSubP1 · nSubP2 · nPatch1 · nPatch2` multiscale spatial grid on the `nPatch1 · nPatch2` array of patches.

- `patches` a struct set by `configPatches2()` which includes the following information.

  - `.x` is `nSubP1`$\times 1 \times 1 \times 1 \times$`nPatch1`$\times 1$ array of the spatial locations x_{iI} of the microscale grid points in every patch. Currently it *must* be an equi-spaced lattice on the microscale index i, but may be variable spaced in macroscale index I.
  - `.y` is similarly $1 \times$ `nSubP2` $\times 1 \times 1 \times 1 \times$ `nPatch2` array of the spatial locations y_{jJ} of the microscale grid points in every patch. Currently it *must* be an equi-spaced lattice on the microscale index j, but may be variable spaced in macroscale index J.
  - `.ordCC` is order of interpolation, currently only $\{0, 2, 4, \ldots\}$
  - `.periodic` indicates whether macroscale is periodic domain, or alternatively that the macroscale has left, right, top and bottom boundaries so interpolation is via divided differences.
  - `.stag` in $\{0, 1\}$ is one for staggered grid (alternating) interpolation. Currently must be zero.
  - `.Cwtsr` and `.Cwtsl` are the coupling coefficients for finite width interpolation in both the x, y-directions—when invoking a periodic domain.
  - `.EdgyInt`, true/false, for determining patch-edge values by interpolation: true, from opposite-edge next-to-edge values (often preserves symmetry); false, from centre cross-patch values (near original scheme).
  - `.nEnsem` the number of realisations in the ensemble.
  - `.parallel` whether serial or parallel.

Output

- `u` is 6D array, `nSubP1 · nSubP2 · nVars · nEnsem · nPatch1 · nPatch2`, of the fields with edge values set by interpolation.

Test for reality of the field values, and define a function accordingly. Could be problematic if some variables are real and some are complex, or if variables are of quite different sizes.

```
117   if max(abs(imag(u(:))))<1e-9*max(abs(u(:)))
118        uclean=@(u) real(u);
119   else uclean=@(u) u;
120   end
```

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

```
128 [~,ny,~,~,~,Ny] = size(patches.y);
129 [nx,~,~,~,Nx,~] = size(patches.x);
130 nEnsem = patches.nEnsem;
131 nVars = round(numel(u)/numel(patches.x)/numel(patches.y)/nEnsem);
132 assert(numel(u) == nx*ny*Nx*Ny*nVars*nEnsem ...
133   ,'patchEdgeInt2: input u has wrong size for parameters')
134 u = reshape(u,[nx ny nVars nEnsem Nx Ny ]);
```

For the moment assume the physical domain is either macroscale periodic or macroscale rectangle so that the coupling formulas are simplest. These index vectors point to patches and, if periodic, their four immediate neighbours.

```
144 I=1:Nx; Ip=mod(I,Nx)+1; Im=mod(I-2,Nx)+1;
145 J=1:Ny; Jp=mod(J,Ny)+1; Jm=mod(J-2,Ny)+1;
```

The centre of each patch (as `nx` and `ny` are odd for centre-patch interpolation) is at indices

```
152 i0 = round((nx+1)/2);
153 j0 = round((ny+1)/2);
```

15.1 Periodic macroscale interpolation schemes

```
162 if patches.periodic
```

Get the size ratios of the patches.

```
168 rx = patches.ratio(1);
169 ry = patches.ratio(2);
```

15.1.1 Lagrange interpolation gives patch-edge values

Compute centred differences of the mid-patch values for the macro-interpolation, of all fields. Here the domain is macro-periodic.

```
ordCC = patches.ordCC;
if ordCC>0 % then finite-width polynomial interpolation
```

Interpolate the three directions in succession, in this way we naturally fill-in corner values. Start with x-direction, and give most documentation for that case as the y-direction is essentially the same.

x-normal edge values The patch-edge values are either interpolated from the next-to-edge values, or from the centre-cross values (not the patch-centre value itself as that seems to have worse properties in general). Have not yet implemented core averages.

```
  if patches.EdgyInt % interpolate next-to-face values
    U = u([2 nx-1],2:(ny-1),:,:,I,J);
  else % interpolate centre-cross values
    U = u(i0,2:(ny-1),:,:,I,J);
  end;%if patches.EdgyInt
```

Just in case the last array dimension(s) are one, we have to force a padding of the sizes, then adjoin the extra dimension for the subsequent array of differences.

```
szU0=size(U); szU0=[szU0 ones(1,6-length(szU0)) ordCC];
```

Use finite difference formulas for the interpolation, so store finite differences $(\mu\delta, \delta^2, \mu\delta^3, \delta^4, \ldots)$ in these arrays. When parallel, in order to preserve the distributed array structure we use an index at the end for the differences.

```
  if ~patches.parallel, dmu = zeros(szU0); % 7D
  else   dmu = zeros(szU0,patches.codist); % 7D
  end%if patches.parallel
```

First compute differences $\mu\delta$ and δ^2.

```
  if patches.stag % use only odd numbered neighbours
    error('polynomial interpolation not yet for staggered patch coupl
%    dmux(:,:,:,:,I,:,1) = (Ux(:,:,:,:,Ip,:)+Ux(:,:,:,:,Im,:))/2; % \
%    dmux(:,:,:,:,I,:,2) = (Ux(:,:,:,:,Ip,:)-Ux(:,:,:,:,Im,:)); % \de
```

```
%    Ip = Ip(Ip); Im = Im(Im); % increase shifts to \pm2
%    dmuy(:,:,:,:,:,J,1) = (Ux(:,:,:,:,:,Jp)+Ux(:,:,:,:,:,Jm))/2; % \
%    dmuy(:,:,:,:,:,J,2) = (Ux(:,:,:,:,:,Jp)-Ux(:,:,:,:,:,Jm)); % \de
%    Jp = Jp(Jp); Jm = Jm(Jm); % increase shifts to \pm2
  else %disp('starting standard interpolation')
    dmu(:,:,:,:,I,:,1) = (U(:,:,:,:,Ip,:) ...
                          -U(:,:,:,:,Im,:))/2; %\mu\delta
    dmu(:,:,:,:,I,:,2) = (U(:,:,:,:,Ip,:) ...
       -2*U(:,:,:,:,I,:) +U(:,:,:,:,Im,:));   %\delta^2
  end% if patches.stag
```

Recursively take δ^2 of these to form successively higher order centred differences in space.

```
  for k = 3:ordCC
    dmu(:,:,:,:,I,:,k) =     dmu(:,:,:,:,Ip,:,k-2) ...
    -2*dmu(:,:,:,:,I,:,k-2) +dmu(:,:,:,:,Im,:,k-2);
  end
```

Interpolate macro-values to be Dirichlet edge values for each patch (Roberts and Kevrekidis 2007; Bunder, Roberts, and Kevrekidis 2017), using weights computed in `configPatches2()`. Here interpolate to specified order.

For the case where next-to-edge values interpolate to the opposite edge-values: when we have an ensemble of configurations, different configurations might be coupled to each other, as specified by `patches.le`, `patches.ri`, `patches.to` and `patches.bo`.

```
k=1+patches.EdgyInt; % use centre or two edges
u(nx,2:(ny-1),:,patches.ri,I,:) ...
  = U(1,:,:,:,:,:)*(1-patches.stag) ...
  +sum( shiftdim(patches.Cwtsr(:,1),-6).*dmu(1,:,:,:,:,:,:) ,7);
u(1 ,2:(ny-1),:,patches.le,I,:,:) ...
  = U(k,:,:,:,:,:)*(1-patches.stag) ...
  +sum( shiftdim(patches.Cwtsl(:,1),-6).*dmu(k,:,:,:,:,:,:) ,7);
```

y-normal edge values Interpolate from either the next-to-edge values, or the centre-cross-line values.

```
  if patches.EdgyInt % interpolate next-to-face values
    U = u(:,[2 ny-1],:,:,I,J);
  else % interpolate centre-cross values
```

```
285       U = u(:,j0,:,:,I,J);
286     end;%if patches.EdgyInt
```

Adjoin extra dimension for the array of differences.

```
292 szUO=size(U); szUO=[szUO ones(1,6-length(szUO)) ordCC];
```

Store finite differences $(\mu\delta, \delta^2, \mu\delta^3, \delta^4, \ldots)$ in this array.

```
299     if ~patches.parallel, dmu = zeros(szUO); % 7D
300     else   dmu = zeros(szUO,patches.codist); % 7D
301     end%if patches.parallel
```

First compute differences $\mu\delta$ and δ^2.

```
307     if patches.stag % use only odd numbered neighbours
308       error('polynomial interpolation not yet for staggered patch coupl
309     else  %disp('starting standard interpolation')
310       dmu(:,:,:,:,:,J,1) = (U(:,:,:,:,:,Jp) ...
311                             -U(:,:,:,:,:,Jm))/2; %\mu\delta
312       dmu(:,:,:,:,:,J,2) = (U(:,:,:,:,:,Jp) ...
313          -2*U(:,:,:,:,:,J) +U(:,:,:,:,:,Jm));   %\delta^2
314     end% if stag
```

Recursively take δ^2.

```
320     for k = 3:ordCC
321       dmu(:,:,:,:,:,J,k) =     dmu(:,:,:,:,:,Jp,k-2) ...
322       -2*dmu(:,:,:,:,:,J,k-2) +dmu(:,:,:,:,:,Jm,k-2);
323     end
```

Interpolate macro-values using the weights pre-computed by `configPatches2()`. An ensemble of configurations may have cross-coupling.

```
331 k = 1+patches.EdgyInt; % use centre or two edges
332 u(:,ny,:,patches.to,:,J) ...
333   = U(:,1,:,:,:,:)*(1-patches.stag) ...
334   +sum( shiftdim(patches.Cwtsr(:,2),-6).*dmu(:,1,:,:,:,:,:) ,7);
335 u(:,1 ,:,patches.bo,:,J) ...
336   = U(:,k,:,:,:,:)*(1-patches.stag) ...
337   +sum( shiftdim(patches.Cwtsl(:,2),-6).*dmu(:,k,:,:,:,:,:) ,7);
```

15.1.2 Case of spectral interpolation

Assumes the domain is macro-periodic.

```
348 else% patches.ordCC<=0, spectral interpolation
```

We interpolate in terms of the patch index, j say, not directly in space. As the macroscale fields are N-periodic in the patch index I, the macroscale Fourier transform writes the centre-patch values as $U_I = \sum_k C_k e^{ik2\pi I/N}$. Then the edge-patch values $U_{I\pm r} = \sum_k C_k e^{ik2\pi/N(I\pm r)} = \sum_k C'_k e^{ik2\pi I/N}$ where $C'_k = C_k e^{ikr2\pi/N}$. For N patches we resolve 'wavenumbers' $|k| < N/2$, so set row vector `ks` $= k2\pi/N$ for 'wavenumbers' $k = (0\,, 1\,, \ldots, k_{\max}\,, -k_{\max}\,, \ldots, -1)$ for odd N, and $k = (0\,, 1\,, \ldots, k_{\max}\,, \pm(k_{\max}+1) - k_{\max}\,, \ldots, -1)$ for even N.

Deal with staggered grid by doubling the number of fields and halving the number of patches (`configPatches2` 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.

```
371  if patches.stag % transform by doubling the number of fields
372  error('staggered grid not yet implemented??')
373    v=nan(size(u)); % currently to restore the shape of u
374    u=cat(3,u(:,1:2:nPatch,:),u(:,2:2:nPatch,:));
375    stagShift=reshape(0.5*[ones(nVars,1);-ones(nVars,1)],1,1,[]);
376    iV=[nVars+1:2*nVars 1:nVars]; % scatter interp to alternate field
377    r=r/2;           % ratio effectively halved
378    nPatch=nPatch/2; % halve the number of patches
379    nVars=nVars*2;   % double the number of fields
380  else % the values for standard spectral
381     stagShift = 0;
382     iV = 1:nVars;
383  end%if patches.stag
```

Interpolate the two directions in succession, in this way we naturally fill-in edge-corner values. Start with x-direction, and give most documentation for that case as the other is essentially the same. Need these indices of patch interior.

```
393 ix = 2:nx-1;   iy = 2:ny-1;
```

x-normal edge values Now set wavenumbers into a vector at the correct dimension. In the case of even N these compute the +-case for the highest wavenumber zig-zag mode, $k = (0\,, 1\,, \ldots, k_{\max}\,, +(k_{\max}+1) - k_{\max}\,, \ldots, -1)$.

```
406   kMax = floor((Nx-1)/2);
407   kr = shiftdim( rx*2*pi/Nx*(mod((0:Nx-1)+kMax,Nx)-kMax) ,-3);
```

Compute the Fourier transform of the centre-cross values. Unless doing patch-edgy interpolation when FT the next-to-edge values. If there are an even number of points, then if complex, treat as positive wavenumber, but if real, treat as cosine. When using an ensemble of configurations, different configurations might be coupled to each other, as specified by `patches.le`, `patches.ri`, `patches.to` and `patches.bo`.

```
420 if ~patches.EdgyInt
421      Cm = fft( u(i0,iy,:,:,:,:) ,[],5);
422      Cp = Cm;
423 else
424      Cm = fft( u(   2,iy ,:,patches.le,:,:) ,[],5);
425      Cp = fft( u(nx-1,iy ,:,patches.ri,:,:) ,[],5);
426 end%if ~patches.EdgyInt
```

Now invert the Fourier transforms to complete interpolation. Enforce reality when appropriate.

```
433 u(nx,iy,:,:,:,:) = uclean( ifft( ...
434     Cm.*exp(1i*(stagShift+kr))  ,[],5) );
435 u( 1,iy,:,:,:,:) = uclean( ifft( ...
436     Cp.*exp(1i*(stagShift-kr))  ,[],5) );
```

y-normal edge values Set wavenumbers into a vector.

```
446   kMax = floor((Ny-1)/2);
447   kr = shiftdim( ry*2*pi/Ny*(mod((0:Ny-1)+kMax,Ny)-kMax) ,-4);
```

Compute the Fourier transform of the patch values on the centre-lines for all the fields.

```
454 if ~patches.EdgyInt
455      Cm = fft( u(:,j0,:,:,:,:) ,[],6);
456      Cp = Cm;
457 else
458      Cm = fft( u(:,2    ,:,patches.bo,:,:) ,[],6);
459      Cp = fft( u(:,ny-1 ,:,patches.to,:,:) ,[],6);
460 end%if ~patches.EdgyInt
```

Invert the Fourier transforms to complete interpolation.

```
u(:,ny,:,:,:,:) = uclean( ifft( ...
    Cm.*exp(1i*(stagShift+kr))  ,[],6) );
u(:, 1,:,:,:,:) = uclean( ifft( ...
    Cp.*exp(1i*(stagShift-kr))  ,[],6) );

end% if ordCC>0 else, so spectral
```

15.2 Non-periodic macroscale interpolation

```
else% patches.periodic false
assert(~patches.stag, ...
'not yet implemented staggered grids for non-periodic')
```

Determine the order of interpolation `px` and `py` (potentially different in the different directions!), and hence size of the (forward) divided difference tables in `F` (7D) for interpolating to left/right, and top/bottom edges. Because of the product-form of the patch grid, and because we are doing *only* either edgy interpolation or cross-patch interpolation (*not* just the centre patch value), the interpolations are all 1D interpolations.

```
if patches.ordCC<1
     px = Nx-1; py = Ny-1;
else px = min(patches.ordCC,Nx-1);
     py = min(patches.ordCC,Ny-1);
end
ix=2:nx-1;  iy=2:ny-1; % indices of edge 'interior' (ix n/a)
```

15.2.1 x-direction values

Set function values in first 'column' of the tables for every variable and across ensemble. For `EdgyInt`, the 'reversal' of the next-to-edge values are because their values are to interpolate to the opposite edge of each patch. [20]

```
  F = nan(patches.EdgyInt+1,ny-2,nVars,nEnsem,Nx,Ny,px+1);
  if patches.EdgyInt % interpolate next-to-edge values
    F(:,:,:,:,:,:,1) = u([nx-1 2],iy,:,:,:,:);
    X = patches.x([nx-1 2],:,:,:,:,:);
```

[20] **ToDo:** Have no plans to implement core averaging as yet.

```
524   else % interpolate mid-patch cross-patch values
525     F(:,:,:,:,:,:,1) = u(i0,iy,:,:,:,:);
526     X = patches.x(i0,:,:,:,:,:);
527   end%if patches.EdgyInt
```

Form tables of divided differences Compute tables of (forward) divided differences (e.g., Wikipedia 2022) for every variable, and across ensemble, and for left/right edges. Recursively find all divided differences.

```
538 for q = 1:px
539   i = 1:Nx-q;
540   F(:,:,:,:,i,:,q+1) ...
541   = (F(:,:,:,:,i+1 ,:,q)-F(:,:,:,:,i,:,q)) ...
542   ./(X(:,:,:,:,i+q,:)   -X(:,:,:,:,i,:));
543 end
```

Interpolate with divided differences Now interpolate to find the edge-values on left/right edges at `Xedge` for every interior `Y`.

```
552 Xedge = patches.x([1 nx],:,:,:,:,:);
```

Code Horner's recursive evaluation of the interpolation polynomials. Indices `i` are those of the left edge of each interpolation stencil, because the table is of forward differences. This alternative: the case of order p_x and p_y interpolation across the domain, asymmetric near the boundaries of the rectangular domain.

```
563   i = max(1,min(1:Nx,Nx-ceil(px/2))-floor(px/2));
564   Uedge = F(:,:,:,:,i,:,px+1);
565   for q = px:-1:1
566     Uedge = F(:,:,:,:,i,:,q)+(Xedge-X(:,:,:,:,i+q-1,:)).*Uedge;
567   end
```

Finally, insert edge values into the array of field values, using the required ensemble shifts.

```
575 u(1 ,iy,:,patches.le,:,:) = Uedge(1,:,:,:,:,:);
576 u(nx,iy,:,patches.ri,:,:) = Uedge(2,:,:,:,:,:);
```

15.2.2 y-direction values

Set function values in first 'column' of the tables for every variable and across ensemble.

```
  F = nan(nx,patches.EdgyInt+1,nVars,nEnsem,Nx,Ny,py+1);
  if patches.EdgyInt % interpolate next-to-edge values
    F(:,:,:,:,:,:,1) = u(:,[ny-1 2],:,:,:,:);
    Y = patches.y(:,[ny-1 2],:,:,:,:);
  else % interpolate mid-patch cross-patch values
    F(:,:,:,:,:,:,1) = u(:,j0,:,:,:,:);
    Y = patches.y(:,j0,:,:,:,:);
  end;
```

Form tables of divided differences.

```
for q = 1:py
  j = 1:Ny-q;
  F(:,:,:,:,:,j,q+1) ...
  = (F(:,:,:,:,:,j+1 ,q)-F(:,:,:,:,:,j,q)) ...
  ./(Y(:,:,:,:,:,j+q)   -Y(:,:,:,:,:,j));
end
```

Interpolate to find the edge-values on top/bottom edges `Yedge` for every x.

```
Yedge = patches.y(:,[1 ny],:,:,:,:);
```

Code Horner's recursive evaluation of the interpolation polynomials. Indices `j` are those of the bottom edge of each interpolation stencil, because the table is of forward differences.

```
  j = max(1,min(1:Ny,Ny-ceil(py/2))-floor(py/2));
  Uedge = F(:,:,:,:,:,j,py+1);
  for q = py:-1:1
    Uedge = F(:,:,:,:,:,j,q)+(Yedge-Y(:,:,:,:,:,j+q-1)).*Uedge;
  end
```

Finally, insert edge values into the array of field values, using the required ensemble shifts.

```
u(:,1 ,:,patches.bo,:,:) = Uedge(:,1,:,:,:,:);
u(:,ny,:,patches.to,:,:) = Uedge(:,2,:,:,:,:);
```

15.2.3 Optional NaNs for safety

We want a user to set outer edge values on the extreme patches according to the microscale boundary conditions that hold at the extremes of the domain. Consequently, override their computed interpolation values with `NaN`.

```
643 u( 1,:,:,:, 1,:) = nan;
644 u(nx,:,:,:,Nx,:) = nan;
645 u(:, 1,:,:,:, 1) = nan;
646 u(:,ny,:,:,:,Ny) = nan;
```

End of the non-periodic interpolation code.

```
653 end%if patches.periodic else
```

Fin, returning the 6D array of field values with interpolated edges.

```
662 end% function patchEdgeInt2
```

16 configPatches2(): configures spatial patches in 2D

Makes the struct `patches` for use by the patch/gap-tooth time derivative/step function `patchSys2()`. Section 16.1 lists an example of its use.

```
19 function patches = configPatches2(fun,Xlim,Dom ...
20     ,nPatch,ordCC,dx,nSubP,varargin)
```

Input If invoked with no input arguments, then executes an example of simulating a nonlinear diffusion PDE relevant to the lubrication flow of a thin layer of fluid—see Section 16.1 for an example code.

- `fun` is the name of the user function, `fun(t,u,patches)` or `fun(t,u)`, that computes time-derivatives (or time-steps) of quantities on the 2D micro-grid within all the 2D patches.
- `Xlim` array/vector giving the rectangular macro-space domain of the computation, namely $[\texttt{Xlim(1)}, \texttt{Xlim(2)}] \times [\texttt{Xlim(3)}, \texttt{Xlim(4)}]$. If `Xlim` has two elements, then the domain is the square domain of the same interval in both directions.
- `Dom` sets the type of macroscale conditions for the patches, and reflects the type of microscale boundary conditions of the problem. If `Dom` is `NaN` or `[]`, then the field `u` is doubly macro-periodic in the 2D spatial domain, and resolved on equi-spaced patches. If `Dom` is a character string, then that specifies the `.type` of the following structure, with `.bcOffset` set to the default zero. Otherwise `Dom` is a structure with the following components.

- `.type`, string, of either `'periodic'` (the default), `'equispace'`, `'chebyshev'`, `'usergiven'`. For all cases except `'periodic'`, users *must* code into `fun` the micro-grid boundary conditions that apply at the left/right/bottom/top edges of the leftmost/rightmost/bottommost/topmost patches, respectively.
- `.bcOffset`, optional one, two or four element vector/array, in the cases of `'equispace'` or `'chebyshev'` the patches are placed so the left/right/top/bottom macroscale boundaries are aligned to the left/right/top/bottom edges of the corresponding extreme patches, but offset by `.bcOffset` of the sub-patch micro-grid spacing. For example, use `bcOffset=0` when the micro-code applies Dirichlet boundary values on the extreme edge micro-grid points, whereas use `bcOffset=0.5` when the microcode applies Neumann boundary conditions halfway between the extreme edge micro-grid points. Similarly for the top and bottom edges.

  If `.bcOffset` is a scalar, then apply the same offset to all boundaries. If two elements, then apply the first offset to both x-boundaries, and the second offset to both y-boundaries. If four elements, then apply the first two offsets to the respective x-boundaries, and the last two offsets to the respective y-boundaries.
- `.X`, optional vector/array with `nPatch(1)` elements, in the case `'usergiven'` it specifies the x-locations of the centres of the patches—the user is responsible the locations makes sense.
- `.Y`, optional vector/array with `nPatch(2)` elements, in the case `'usergiven'` it specifies the y-locations of the centres of the patches—the user is responsible the locations makes sense.

- `nPatch` sets the number of equi-spaced spatial patches: if scalar, then use the same number of patches in both directions, otherwise `nPatch(1:2)` gives the number of patches (≥ 1) in each direction.

- `ordCC` is the 'order' of interpolation for inter-patch coupling across empty space of the macroscale patch values to the edge-values of the patches: currently must be $0, 2, 4, \ldots$; where 0 gives spectral interpolation.

- `dx` (real—scalar or two element) is usually the sub-patch micro-grid spacing in x and y. If scalar, then use the same `dx` in both directions, otherwise `dx(1:2)` gives the spacing in each of the two directions.

However, if `Dom` is `NaN` (as for pre-2023), then `dx` actually is `ratio` (scalar or two element), namely the ratio of (depending upon `EdgyInt`) either the half-width or full-width of a patch to the equi-spacing of the patch mid-points. So either `ratio` $= \frac{1}{2}$ means the patches abut and `ratio` $= 1$ is overlapping patches as in holistic discretisation, or `ratio` $= 1$ means the patches abut. Small `ratio` should greatly reduce computational time.

- `nSubP` is the number of equi-spaced microscale lattice points in each patch: if scalar, then use the same number in both directions, otherwise `nSubP(1:2)` gives the number in each direction. If not using `EdgyInt`, then must be odd so that there is/are centre-patch micro-grid point/lines in each patch.

- `nEdge` (not yet implemented), *optional*, default=1, for each patch, the number of edge values set by interpolation at the edge regions of each patch. The default is one (suitable for microscale lattices with only nearest neighbour interactions).

- `EdgyInt`, true/false, *optional*, default=false. If true, then interpolate to left/right/top/bottom edge-values from right/left/bottom/top next-to-edge values. If false or omitted, then interpolate from centre cross-patch lines.

- `nEnsem`, *optional-experimental*, default one, but if more, then an ensemble over this number of realisations.

- `hetCoeffs`, *optional*, default empty. Supply a 2D or 3D array of microscale heterogeneous coefficients to be used by the given microscale `fun` in each patch. Say the given array `cs` is of size $m_x \times m_y \times n_c$, where n_c is the number of different sets of coefficients. For example, in heterogeneous diffusion, $n_c = 2$ for the diffusivities in the *two* different spatial directions (or $n_c = 3$ for the diffusivity tensor). The coefficients are to be the same for each and every patch; however, macroscale variations are catered for by the n_c coefficients being n_c parameters in some macroscale formula.

  - If `nEnsem` $= 1$, then the array of coefficients is just tiled across the patch size to fill up each patch, starting from the $(1, 1)$-point in each patch.
  - If `nEnsem` > 1 (value immaterial), then reset `nEnsem` $:= m_x \cdot m_y$ and construct an ensemble of all $m_x \cdot m_y$ phase-shifts of the coefficients. In this scenario, the inter-patch coupling couples different members

in the ensemble. When `EdgyInt` is true, and when the coefficients are diffusivities/elasticities in x and y directions, respectively, then this coupling cunningly preserves symmetry.

- `'parallel'`, true/false, *optional*, default=false. If false, then all patch computations are on the user's main CPU—although a user may well separately invoke, say, a GPU to accelerate sub-patch computations.

  If true, and it requires that you have MATLAB's Parallel Computing Toolbox, then it will distribute the patches over multiple CPUs/cores. In MATLAB, only one array dimension can be split in the distribution, so it chooses the one space dimension x, y corresponding to the highest `\nPatch` (if a tie, then chooses the rightmost of x, y). A user may correspondingly distribute arrays with property `patches.codist`, or simply use formulas invoking the preset distributed arrays `patches.x`, and `patches.y`. If a user has not yet established a parallel pool, then a 'local' pool is started.

Output The struct `patches` is created and set with the following components. If no output variable is provided for `patches`, then make the struct available as a global variable.[21]

```
206 if nargout==0, global patches, end
```

- `.fun` is the name of the user's function `fun(t,u,patches)` or `fun(t,u)`, that computes the time derivatives (or steps) on the patchy lattice.
- `.ordCC` is the specified order of inter-patch coupling.
- `.periodic`: either true, for interpolation on the macro-periodic domain; or false, for general interpolation by divided differences over non-periodic domain or unevenly distributed patches.
- `.stag` is true for interpolation using only odd neighbouring patches as for staggered grids, and false for the usual case of all neighbour coupling—not yet implemented.
- `.Cwtsr` and `.Cwtsl`, only for macro-periodic conditions, are the `ordCC`$\times 2$-array of weights for the inter-patch interpolation onto the right/top and

[21] When using `spmd` parallel computing, it is generally best to avoid global variables, and so instead prefer using an explicit output variable.

left/bottom edges (respectively) with patch:macroscale ratio as specified or as derived from `dx`.

- `.x` (6D) is `nSubP(1)` $\times 1 \times 1 \times 1 \times$ `nPatch(1)` $\times 1$ array of the regular spatial locations x_{iI} of the microscale grid points in every patch.
- `.y` (6D) is $1 \times$ `nSubP(2)` $\times 1 \times 1 \times 1 \times$ `nPatch(2)` array of the regular spatial locations y_{jJ} of the microscale grid points in every patch.
- `.ratio` 1×2, only for macro-periodic conditions, are the size ratios of every patch.
- `.nEdge` is, for each patch, the number of edge values set by interpolation at the edge regions of each patch.
- `.le`, `.ri`, `.bo`, `.to` determine inter-patch coupling of members in an ensemble. Each a column vector of length `nEnsem`.
- `.cs` either
  - `[]` 0D, or
  - if `nEnsem` $= 1$, (`nSubP(1)` $- 1$) $\times$ (`nSubP(2)` $- 1$) $\times n_c$ 3D array of microscale heterogeneous coefficients, or
  - if `nEnsem` > 1, (`nSubP(1)` -1) $\times$ (`nSubP(2)` -1) $\times n_c \times m_x m_y$ 4D array of $m_x m_y$ ensemble of phase-shifts of the microscale heterogeneous coefficients.
- `.parallel`, logical: true if patches are distributed over multiple CPUs/ cores for the Parallel Computing Toolbox, otherwise false (the default is to activate the *local* pool).
- `.codist`, *optional*, describes the particular parallel distribution of arrays over the active parallel pool.

16.1 If no arguments, then execute an example

```
289 if nargin==0
290 disp('With no arguments, simulate example of nonlinear diffusion')
```

The code here shows one way to get started: a user's script may have the following three steps (" $\mapsto$ " denotes function recursion).

1. configPatches2

2. ode23 integrator $\mapsto$ patchSys2 $\mapsto$ user's PDE
3. process results

Establish global patch data struct to interface with a function coding a nonlinear 'diffusion' PDE: to be solved on 6×4-periodic domain, with 9×7 patches, spectral interpolation (0) couples the patches, with 5×5 points forming the micro-grid in each patch, and a sub-patch micro-grid spacing of 0.12 (relatively large for visualisation). Roberts, MacKenzie, and Bunder (2014) established that this scheme is consistent with the PDE (as the patch spacing decreases).

```
global patches
patches = configPatches2(@nonDiffPDE,[-3 3 -2 2], [] ...
    , [9 7], 0, 0.12, 5 ,'EdgyInt',false);
```

Set an initial condition of a perturbed-Gaussian using auto-replication of the spatial grid.

```
u0 = exp(-patches.x.^2-patches.y.^2);
u0 = u0.*(0.9+0.1*rand(size(u0)));
```

Initiate a plot of the simulation using only the microscale values interior to the patches: optionally set x and y-edges to `nan` to leave the gaps between patches.

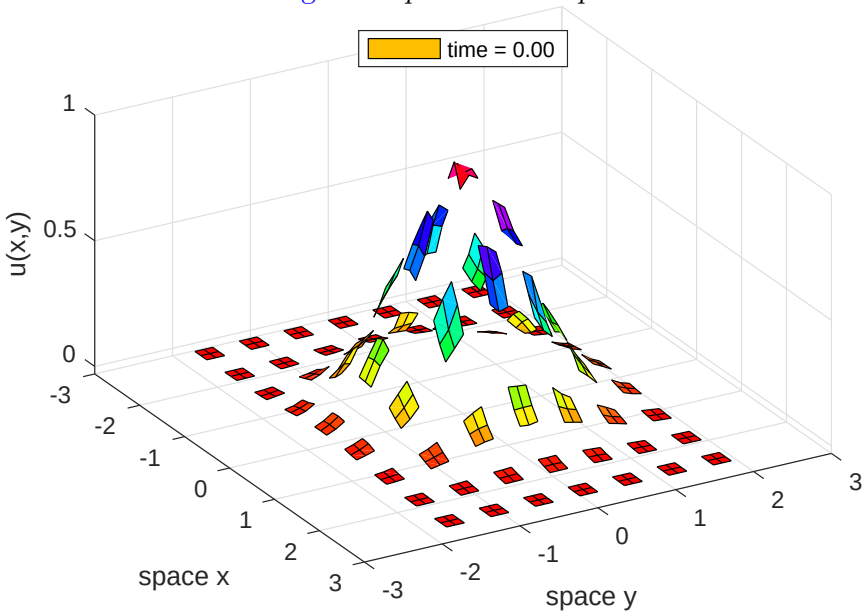
```
figure(1), clf, colormap(0.8*hsv)
x = squeeze(patches.x);  y = squeeze(patches.y);
if 1, x([1 end],:) = nan; y([1 end],:) = nan; end
```

Start by showing the initial conditions of Figure 15 while the simulation computes.

```
u = reshape(permute(squeeze(u0) ...
    ,[1 3 2 4]), [numel(x) numel(y)]);
hsurf = surf(x(:),y(:),u');
axis([-3 3 -3 3 -0.03 1]), view(60,40)
legend('time = 0.00','Location','north')
xlabel('space x'), ylabel('space y'), zlabel('u(x,y)')
colormap(hsv)
ifOurCf2eps([mfilename 'ic'])
```

Integrate in time to $t = 4$ using standard functions. In MATLAB `ode15s` would be natural as the patch scheme is naturally stiff, but `ode23` is quicker (Maclean, Bunder, and Roberts 2021, Fig. 4). Ask for output at non-uniform times because the diffusion slows.

Figure 15: initial field $u(x, y, t)$ at time $t = 0$ of the patch scheme applied to a nonlinear 'diffusion' PDE: Figure 16 plots the computed field at time $t = 3$.

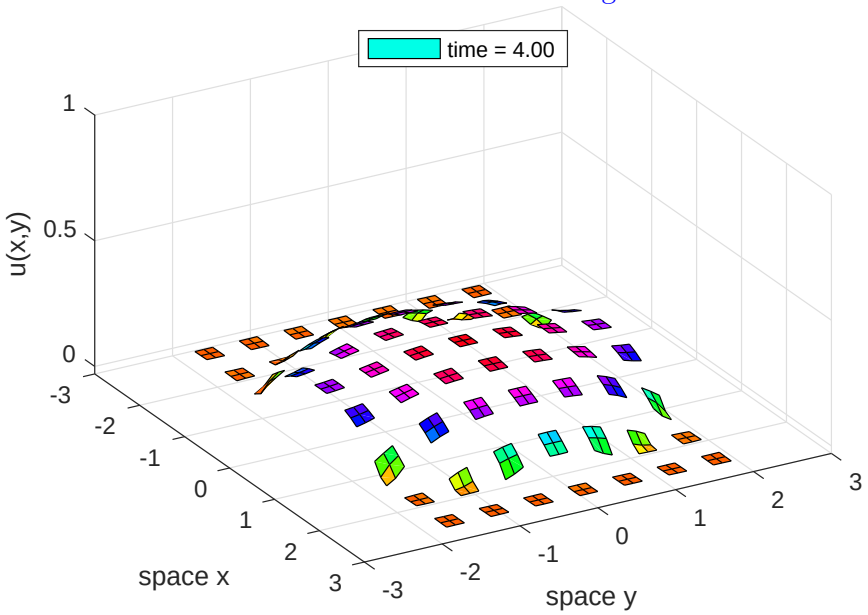



```
disp('Wait to simulate nonlinear diffusion h_t=(h^3)_xx+(h^3)_yy')
drawnow
if ~exist('OCTAVE_VERSION','builtin')
    [ts,us] = ode23(@patchSys2,linspace(0,2).^2,u0(:));
else % octave version is quite slow for me
    lsode_options('absolute tolerance',1e-4);
    lsode_options('relative tolerance',1e-4);
    [ts,us] = odeOcts(@patchSys2,[0 1],u0(:));
end
```

Animate the computed simulation to end with Figure 16. Use `patchEdgeInt2` to interpolate patch-edge values.

```
for i = 1:length(ts)
  u = patchEdgeInt2(us(i,:));
  u = reshape(permute(squeeze(u) ...
      ,[1 3 2 4]), [numel(x) numel(y)]);
  set(hsurf,'ZData', u');
  legend(['time = ' num2str(ts(i),'%4.2f')])
```

Figure 16: field $u(x, y, t)$ at time $t = 3$ of the patch scheme applied to a nonlinear 'diffusion' PDE with initial condition in Figure 15.




```
  pause(0.1)
end
ifOurCf2eps([mfilename 't3'])
```

Upon finishing execution of the example, exit this function.

```
return
end%if no arguments
```

16.2 Parse input arguments and defaults

```
p = inputParser;
fnValidation = @(f) isa(f, 'function_handle');%test for fn name
addRequired(p,'fun',fnValidation);
addRequired(p,'Xlim',@isnumeric);
%addRequired(p,'Dom'); % nothing yet decided
addRequired(p,'nPatch',@isnumeric);
addRequired(p,'ordCC',@isnumeric);
addRequired(p,'dx',@isnumeric);
```

```
addRequired(p,'nSubP',@isnumeric);
addParameter(p,'nEdge',1,@isnumeric);
addParameter(p,'EdgyInt',false,@islogical);
addParameter(p,'nEnsem',1,@isnumeric);
addParameter(p,'hetCoeffs',[],@isnumeric);
addParameter(p,'parallel',false,@islogical);
%addParameter(p,'nCore',1,@isnumeric); % not yet implemented
parse(p,fun,Xlim,nPatch,ordCC,dx,nSubP,varargin{:});
```

Set the optional parameters.

```
patches.nEdge = p.Results.nEdge;
patches.EdgyInt = p.Results.EdgyInt;
patches.nEnsem = p.Results.nEnsem;
cs = p.Results.hetCoeffs;
patches.parallel = p.Results.parallel;
%patches.nCore = p.Results.nCore;
```

Initially duplicate parameters for both space dimensions as needed.

```
if numel(Xlim)==2,   Xlim = repmat(Xlim,1,2); end
if numel(nPatch)==1, nPatch = repmat(nPatch,1,2); end
if numel(dx)==1,     dx = repmat(dx,1,2); end
if numel(nSubP)==1,  nSubP = repmat(nSubP,1,2); end
```

Check parameters.

```
assert(Xlim(1)<Xlim(2) ...
      ,'first pair of Xlim must be ordered increasing')
assert(Xlim(3)<Xlim(4) ...
      ,'second pair of Xlim must be ordered increasing')
assert(patches.nEdge==1 ...
      ,'multi-edge-value interp not yet implemented')
assert(all(2*patches.nEdge<nSubP) ...
      ,'too many edge values requested')
%if patches.nCore>1
%    warning('nCore>1 not yet tested in this version')
%    end
```

For compatibility with pre-2023 functions, if parameter `Dom` is `Nan`, then we set the `ratio` to be the value of the so-called `dx` vector.

```
if ~isstruct(Dom), pre2023=isnan(Dom);
else pre2023=false; end
if pre2023, ratio=dx; dx=nan; end
```

Default macroscale conditions are periodic with evenly spaced patches.

```
if isempty(Dom), Dom=struct('type','periodic'); end
if (~isstruct(Dom))&isnan(Dom), Dom=struct('type','periodic'); end
```

If `Dom` is a string, then just set type to that string, and subsequently set corresponding defaults for others fields.

```
if ischar(Dom), Dom=struct('type',Dom); end
```

We allow different macroscale domain conditions in the different directions. But for the moment do not allow periodic to be mixed with the others (as the interpolation mechanism is different code)—hence why we choose `periodic` be seven characters, whereas the others are eight characters. The different conditions are coded in different rows of `Dom.type`, so we duplicate the string if only one row specified.

```
if size(Dom.type,1)==1, Dom.type=repmat(Dom.type,2,1); end
```

Check what is and is not specified, and provide default of zero (Dirichlet boundaries) if no `bcOffset` specified when needed. Do so for both directions independently.

```
patches.periodic=false;
for p=1:2
switch Dom.type(p,:)
case 'periodic'
    patches.periodic=true;
    if isfield(Dom,'bcOffset')
    warning('bcOffset not available for Dom.type = periodic'), end
    msg=' not available for Dom.type = periodic';
    if isfield(Dom,'X'), warning(['X' msg]), end
    if isfield(Dom,'Y'), warning(['Y' msg]), end
case {'equispace','chebyshev'}
    if ~isfield(Dom,'bcOffset'), Dom.bcOffset=zeros(2,2); end
    % for mixed with usergiven, following should still work
    if numel(Dom.bcOffset)==1
        Dom.bcOffset=repmat(Dom.bcOffset,2,2); end
```

```
    if numel(Dom.bcOffset)==2
        Dom.bcOffset=repmat(Dom.bcOffset(:)',2,1); end
    msg=' not available for Dom.type = equispace or chebyshev';
    if (p==1)& isfield(Dom,'X'), warning(['X' msg]), end
    if (p==2)& isfield(Dom,'Y'), warning(['Y' msg]), end
case 'usergiven'
%    if isfield(Dom,'bcOffset')
%    warning('bcOffset not available for usergiven Dom.type'), end
    msg=' required for Dom.type = usergiven';
    if p==1, assert(isfield(Dom,'X'),['X' msg]), end
    if p==2, assert(isfield(Dom,'Y'),['Y' msg]), end
otherwise
    error([Dom.type 'is unknown Dom.type'])
end%switch Dom.type
end%for p
```

16.3 The code to make patches

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. Spectral coupling is `ordCC` of 0 or (not yet??) -1. [22]

```
assert((ordCC>=-1) & (floor(ordCC)==ordCC), ...
    'ordCC out of allowed range integer>=-1')
```

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

```
patches.stag = mod(ordCC,2);
assert(patches.stag==0,'staggered not yet implemented??')
ordCC = ordCC+patches.stag;
patches.ordCC = ordCC;
```

Check for staggered grid and periodic case.

```
if patches.stag, assert(all(mod(nPatch,2)==0), ...
    'Require an even number of patches for staggered grid')
end
```

[22] **ToDo:** Perhaps implement staggered spectral coupling.

Set the macro-distribution of patches Third, set the centre of the patches in the macroscale grid of patches. Loop over the coordinate directions, setting the distribution into `Q` and finally assigning to array of corresponding direction.

```
for q=1:2
qq=2*q-1;
```

Distribution depends upon `Dom.type`:

```
switch Dom.type(q,:)
```

The periodic case is evenly spaced within the spatial domain. Store the size ratio in `patches`.

```
case 'periodic'
  Q=linspace(Xlim(qq),Xlim(qq+1),nPatch(q)+1);
  DQ=Q(2)-Q(1);
  Q=Q(1:nPatch(q))+diff(Q)/2;
  pEI=patches.EdgyInt;% abbreviation
  if pre2023, dx(q) = ratio(q)*DQ/(nSubP(q)-1-pEI)*(2-pEI);
  else        ratio(q) = dx(q)/DQ*(nSubP(q)-1-pEI)/(2-pEI);
  end
  patches.ratio=ratio;
```

The equi-spaced case is also evenly spaced but with the extreme edges aligned with the spatial domain boundaries, modified by the offset.

```
case 'equispace'
  Q=linspace(Xlim(qq)+((nSubP(q)-1)/2-Dom.bcOffset(qq))*dx(q) ...
          ,Xlim(qq+1)-((nSubP(q)-1)/2-Dom.bcOffset(qq+1))*dx(q) ...
          ,nPatch(q));
  DQ=diff(Q(1:2));
  width=(1+patches.EdgyInt)/2*(nSubP(q)-1-patches.EdgyInt)*dx;
  if DQ<width*0.999999
     warning('too many equispace patches (double overlapping)')
     end
```

The Chebyshev case is spaced according to the Chebyshev distribution in order to reduce macro-interpolation errors, $Q_i \propto -\cos(i\pi/N)$, but with the extreme

edges aligned with the spatial domain boundaries, modified by the offset, and modified by possible 'boundary layers'. [23]

```
case 'chebyshev'
  halfWidth=dx(q)*(nSubP(q)-1)/2;
  Q1 = Xlim(1)+halfWidth-Dom.bcOffset(qq)*dx(q);
  Q2 = Xlim(2)-halfWidth+Dom.bcOffset(qq+1)*dx(q);
%  Q = (Q1+Q2)/2-(Q2-Q1)/2*cos(linspace(0,pi,nPatch));
```

Search for total width of 'boundary layers' so that in the interior the patches are non-overlapping Chebyshev. But the width for assessing overlap of patches is the following variable `width`.

```
  width=(1+patches.EdgyInt)/2*(nSubP(q)-1-patches.EdgyInt)*dx(q);
  for b=0:2:nPatch(q)-2
    DQmin=(Q2-Q1-b*width)/2*( 1-cos(pi/(nPatch(q)-b-1)) );
    if DQmin>width, break, end
  end
  if DQmin<width*0.999999
     warning('too many Chebyshev patches (mid-domain overlap)')
     end
```

Assign the centre-patch coordinates.

```
  Q =[ Q1+(0:b/2-1)*width ...
       (Q1+Q2)/2-(Q2-Q1-b*width)/2*cos(linspace(0,pi,nPatch(q)-b)) ..
       Q2+(1-b/2:0)*width ];
```

The user-given case is entirely up to a user to specify, we just ensure it has the correct shape of a row??.

```
case 'usergiven'
  if q==1, Q = reshape(Dom.X,1,[]);
  else     Q = reshape(Dom.Y,1,[]);
  end%if
end%switch Dom.type
```

Assign Q-coordinates to the correct spatial direction. At this stage they are all rows.

[23] However, maybe overlapping patches near a boundary should be viewed as some sort of spatially analogue of the 'christmas tree' of projective integration and its integration to a slow manifold. Here maybe the overlapping patches allow for a 'christmas tree' approach to the boundary layers. Needs to be explored??

```
if q==1, X=Q; end
if q==2, Y=Q; end
end%for q
```

Construct the micro-grids Fourth, construct the microscale grid in each patch. Reshape the grid to be 6D to suit dimensions (micro,Vars,Ens,macro).

```
nSubP = reshape(nSubP,1,2); % force to be row vector
assert(patches.EdgyInt | all(mod(nSubP,2)==1), ...
    'configPatches2: nSubP must be odd')
i0 = (nSubP(1)+1)/2;
patches.x = reshape( dx(1)*(-i0+1:i0-1)'+X ...
                    ,nSubP(1),1,1,1,nPatch(1),1);
```

Next the y-direction.

```
i0 = (nSubP(2)+1)/2;
patches.y = reshape( dx(2)*(-i0+1:i0-1)'+Y ...
                    ,1,nSubP(2),1,1,1,nPatch(2));
```

Pre-compute weights for macro-periodic In the case of macro-periodicity, precompute the weightings to interpolate field values for coupling. [24]

```
if patches.periodic
  ratio = reshape(ratio,1,2); % force to be row vector
  patches.ratio=ratio;
  if ordCC>0
    [Cwtsr,Cwtsl] = patchCwts(ratio,ordCC,patches.stag);
    patches.Cwtsr = Cwtsr;  patches.Cwtsl = Cwtsl;
  end%if
end%if patches.periodic
```

16.4 Set ensemble inter-patch communication

For `EdgyInt` or centre interpolation respectively,

- the right-edge/centre realisations `1:nEnsem` are to interpolate to left-edge `le`, and
- the left-edge/centre realisations `1:nEnsem` are to interpolate to `re`.

[24] **ToDo:** Might sometime extend to coupling via derivative values.

`re` and `li` are 'transposes' of each other as `re(li)=le(ri)` are both `1:nEnsem`. Similarly for bottom-edge/centre interpolation to top-edge via `to`, and top-edge/centre interpolation to bottom-edge via `bo`.

The default is nothing shifty. This setting reduces the number of if-statements in function `patchEdgeInt2()`.

```
788 nE = patches.nEnsem;
789 patches.le = 1:nE;  patches.ri = 1:nE;
790 patches.bo = 1:nE;  patches.to = 1:nE;
```

However, if heterogeneous coefficients are supplied via `hetCoeffs`, then do some non-trivial replications. First, get microscale periods, patch size, and replicate many times in order to subsequently sub-sample: `nSubP` times should be enough. If `cs` is more then 3D, then the higher-dimensions are reshaped into the 3rd dimension.

```
802 if ~isempty(cs)
803   [mx,my,nc] = size(cs);
804   nx = nSubP(1); ny = nSubP(2);
805   cs = repmat(cs,nSubP);
```

If only one member of the ensemble is required, then sub-sample to patch size, and store coefficients in `patches` as is.

```
813   if nE==1, patches.cs = cs(1:nx-1,1:ny-1,:); else
```

But for `nEnsem` > 1 an ensemble of $m_x m_y$ phase-shifts of the coefficients is constructed from the over-supply. Here code phase-shifts over the periods—the phase shifts are like Hankel-matrices.

```
822     patches.nEnsem = mx*my;
823     patches.cs = nan(nx-1,ny-1,nc,mx,my);
824     for j = 1:my
825         js = (j:j+ny-2);
826         for i = 1:mx
827             is = (i:i+nx-2);
828             patches.cs(:,:,:,i,j) = cs(is,js,:);
829         end
830     end
831     patches.cs = reshape(patches.cs,nx-1,ny-1,nc,[]);
```

Further, set a cunning left/right/bottom/top realisation of inter-patch coupling. The aim is to preserve symmetry in the system when also invoking `EdgyInt`. What this coupling does without `EdgyInt` is unknown. Use auto-replication.

```
841     le = mod((0:mx-1)+mod(nx-2,mx),mx)+1;
842     patches.le = reshape(  le'+mx*(0:my-1)  ,[],1);
843     ri = mod((0:mx-1)-mod(nx-2,mx),mx)+1;
844     patches.ri = reshape(  ri'+mx*(0:my-1)  ,[],1);
845     bo = mod((0:my-1)+mod(ny-2,my),my)+1;
846     patches.bo = reshape( (1:mx)'+mx*(bo-1) ,[],1);
847     to = mod((0:my-1)-mod(ny-2,my),my)+1;
848     patches.to = reshape( (1:mx)'+mx*(to-1) ,[],1);
```

Issue warning if the ensemble is likely to be affected by lack of scale separation. [25]

```
856 if prod(ratio)*patches.nEnsem>0.9, warning( ...
857 'Probably poor scale separation in ensemble of coupled phase-shifts')
858 scaleSeparationParameter = ratio*patches.nEnsem
859 end
```

End the two if-statements.

```
865   end%if-else nEnsem>1
866 end%if not-empty(cs)
```

If parallel code then first assume this is not within an `spmd`-environment, and so we invoke `spmd...end` (which starts a parallel pool if not already started). At this point, the global `patches` is copied for each worker processor and so it becomes *composite* when we distribute any one of the fields. Hereafter, *all fields in the global variable* `patches` *must only be referenced within an* `spmd`*-environment.*[26]

```
885 if patches.parallel
886 %  theparpool=gcp()
887   spmd
```

Second, decide which dimension is to be sliced among parallel workers (for the moment, do not consider slicing the ensemble). Choose the direction of most patches, biased towards the last.

[25] **ToDo:** Maybe need to justify this and the arbitrary threshold more carefully??

[26] If subsequently outside spmd, then one must use functions like `getfield(patches{1},'a')`.

```
  [~,pari]=max(nPatch+0.01*(1:2));
  patches.codist=codistributor1d(4+pari);
```

`patches.codist.Dimension` is the index that is split among workers. Then distribute the appropriate coordinate direction among the workers: the function must be invoked inside an `spmd`-group in order for this to work—so we do not need `parallel` in argument list.

```
  switch pari
    case 1, patches.x=codistributed(patches.x,patches.codist);
    case 2, patches.y=codistributed(patches.y,patches.codist);
  otherwise
    error('should never have bad index for parallel distribution')
  end%switch
  end%spmd
```

If not parallel, then clean out `patches.codist` if it exists. May not need, but safer.

```
else% not parallel
  if isfield(patches,'codist'), rmfield(patches,'codist'); end
end%if-parallel
```

Fin

```
end% function
```

17 patchEdgeInt3(): sets 3D patch face values from 3D macroscale interpolation

Couples 3D patches across 3D space by computing their face values via macroscale interpolation. Assumes patch face values are determined by macroscale interpolation of the patch centre-plane values (Roberts, MacKenzie, and Bunder 2014; Bunder et al. 2021), or patch next-to-face values which appears better (Bunder, Kevrekidis, and Roberts 2021). This function is primarily used by `patchSys3()` but is also useful for user graphics. [27]

Communicate patch-design variables via a second argument (optional, except required for parallel computing of `spmd`), or otherwise via the global struct `patches`.

[27] Script `patchEdgeInt3test.m` verifies this code.

```
function u = patchEdgeInt3(u,patches)
if nargin<2, global patches, end
```

Input

- `u` is a vector/array of length `prod(nSubP)·nVars·nEnsem·prod(nPatch)` where there are `nVars · nEnsem` field values at each of the points in the `nSubP1 · nSubP2 · nSubP3 · nPatch1 · nPatch2 · nPatch3` multiscale spatial grid on the `nPatch1 · nPatch2 · nPatch3` array of patches.
- `patches` a struct set by `configPatches3()` which includes the following information.
  - `.x` is `nSubP1` $\times 1 \times 1 \times 1 \times 1 \times$ `nPatch1` $\times 1 \times 1$ array of the spatial locations x_{iI} of the microscale grid points in every patch. Currently it *must* be an equi-spaced lattice on the microscale index i, but may be variable spaced in macroscale index I.
  - `.y` is similarly $1 \times$ `nSubP2` $\times 1 \times 1 \times 1 \times 1 \times$ `nPatch2` $\times 1$ array of the spatial locations y_{jJ} of the microscale grid points in every patch. Currently it *must* be an equi-spaced lattice on the microscale index j, but may be variable spaced in macroscale index J.
  - `.z` is similarly $1 \times 1 \times$ `nSubP3` $\times 1 \times 1 \times 1 \times 1 \times$ `nPatch3` array of the spatial locations z_{kK} of the microscale grid points in every patch. Currently it *must* be an equi-spaced lattice on the microscale index k, but may be variable spaced in macroscale index K.
  - `.ordCC` is order of interpolation, currently only $\{0, 2, 4, \ldots\}$
  - `.periodic` indicates whether macroscale is periodic domain, or alternatively that the macroscale has left, right, top, bottom, front and back boundaries so interpolation is via divided differences.
  - `.stag` in $\{0, 1\}$ is one for staggered grid (alternating) interpolation. Currently must be zero.
  - `.Cwtsr` and `.Cwtsl` are the coupling coefficients for finite width interpolation in each of the x, y, z-directions—when invoking a periodic domain.
  - `.EdgyInt`, true/false, for determining patch-edge values by interpolation: true, from opposite-edge next-to-edge values (often preserves symmetry); false, from centre cross-patch values (near original scheme).

– `.nEnsem` the number of realisations in the ensemble.
– `.parallel` whether serial or parallel.

Output

- `u` is 8D array, `nSubP1·nSubP2·nSubP3·nVars·nEnsem·nPatch1·nPatch2·nPatch3`, of the fields with face values set by interpolation.

Test for reality of the field values, and define a function accordingly. Could be problematic if some variables are real and some are complex, or if variables are of quite different sizes.

```
124   if max(abs(imag(u(:))))<1e-9*max(abs(u(:)))
125        uclean=@(u) real(u);
126   else uclean=@(u) u;
127   end
```

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

```
135 [~,~,nz,~,~,~,~,Nz] = size(patches.z);
136 [~,ny,~,~,~,~,Ny,~] = size(patches.y);
137 [nx,~,~,~,~,Nx,~,~] = size(patches.x);
138 nEnsem = patches.nEnsem;
139 nVars = round( numel(u)/numel(patches.x) ...
140     /numel(patches.y)/numel(patches.z)/nEnsem );
141 assert(numel(u) == nx*ny*nz*Nx*Ny*Nz*nVars*nEnsem ...
142   ,'patchEdgeInt3: input u has wrong size for parameters')
143 u = reshape(u,[nx ny nz nVars nEnsem Nx Ny Nz]);
```

For the moment assume the physical domain is either macroscale periodic or macroscale rectangle so that the coupling formulas are simplest. These index vectors point to patches and, if periodic, their six immediate neighbours.

```
153 I=1:Nx; Ip=mod(I,Nx)+1; Im=mod(I-2,Nx)+1;
154 J=1:Ny; Jp=mod(J,Ny)+1; Jm=mod(J-2,Ny)+1;
155 K=1:Nz; Kp=mod(K,Nz)+1; Km=mod(K-2,Nz)+1;
```

The centre of each patch (as `nx`, `ny` and `nz` are odd for centre-patch interpolation) is at indices

```
163 i0 = round((nx+1)/2);
164 j0 = round((ny+1)/2);
165 k0 = round((nz+1)/2);
```

17.1 Periodic macroscale interpolation schemes

```
174 if patches.periodic
```

Get the size ratios of the patches in each direction.

```
180 rx = patches.ratio(1);
181 ry = patches.ratio(2);
182 rz = patches.ratio(3);
```

17.1.1 Lagrange interpolation gives patch-face values

Compute centred differences of the mid-patch values for the macro-interpolation, of all fields. Here the domain is macro-periodic.

```
193 ordCC = patches.ordCC;
194 if ordCC>0 % then finite-width polynomial interpolation
```

Interpolate the three directions in succession, in this way we naturally fill-in face-edge and corner values. Start with x-direction, and give most documentation for that case as the others are essentially the same.

x-normal face values The patch-edge values are either interpolated from the next-to-edge-face values, or from the centre-cross-plane values (not the patch-centre value itself as that seems to have worse properties in general). Have not yet implemented core averages.

```
210   if patches.EdgyInt % interpolate next-to-face values
211     U = u([2 nx-1],2:(ny-1),2:(nz-1),:,:,I,J,K);
212   else % interpolate centre-cross values
213     U = u(i0,2:(ny-1),2:(nz-1),:,:,I,J,K);
214   end;%if patches.EdgyInt
```

Just in case the last array dimension(s) are one, we have to force a padding of the sizes, then adjoin the extra dimension for the subsequent array of differences.

```
222 szUO=size(U); szUO=[szUO ones(1,8-length(szUO)) ordCC];
```

Use finite difference formulas for the interpolation, so store finite differences $(\mu\delta, \delta^2, \mu\delta^3, \delta^4, \ldots)$ in these arrays. When parallel, in order to preserve the distributed array structure we use an index at the end for the differences.

```
232   if ~patches.parallel, dmu = zeros(szUO); % 9D
233   else   dmu = zeros(szUO,patches.codist); % 9D
234   end%if patches.parallel
```

First compute differences $\mu\delta$ and δ^2.

```
240   if patches.stag % use only odd numbered neighbours
241     error('polynomial interpolation not yet for staggered patch coupl
242 %     dmux(:,:,:,:,:,I,:,:,1) = (Ux(:,:,:,:,:,Ip,:,:) +Ux(:,:,:,:,:,Im
243 %     dmux(:,:,:,:,:,I,:,:,2) = (Ux(:,:,:,:,:,Ip,:,:) -Ux(:,:,:,:,:,Im
244 %     Ip = Ip(Ip); Im = Im(Im); % increase shifts to \pm2
245 %     dmuy(:,:,:,:,:,:,J,:,1) = (Ux(:,:,:,:,:,:,Jp,:)+Ux(:,:,:,:,:,:,J
246 %     dmuy(:,:,:,:,:,:,J,:,2) = (Ux(:,:,:,:,:,:,Jp,:)-Ux(:,:,:,:,:,:,J
247 %     Jp = Jp(Jp); Jm = Jm(Jm); % increase shifts to \pm2
248 %     dmuz(:,:,:,:,:,:,:,K,1) = (Ux(:,:,:,:,:,:,:,Kp)+Ux(:,:,:,:,:,:,:
249 %     dmuz(:,:,:,:,:,:,:,K,2) = (Ux(:,:,:,:,:,:,:,Kp)-Ux(:,:,:,:,:,:,:
250 %     Kp = Kp(Kp); Km = Km(Km); % increase shifts to \pm2
251   else  %disp('starting standard interpolation')
252     dmu(:,:,:,:,:,I,:,:,1) = (U(:,:,:,:,:,Ip,:,:) ...
253                               -U(:,:,:,:,:,Im,:,:))/2; %\mu\delta
254     dmu(:,:,:,:,:,I,:,:,2) = (U(:,:,:,:,:,Ip,:,:) ...
255        -2*U(:,:,:,:,:,I,:,:) +U(:,:,:,:,:,Im,:,:));   %\delta^2
256   end% if stag
```

Recursively take δ^2 of these to form successively higher order centred differences in space.

```
263   for k = 3:ordCC
264     dmu(:,:,:,:,:,I,:,:,k) =     dmu(:,:,:,:,:,Ip,:,:,k-2) ...
265     -2*dmu(:,:,:,:,:,I,:,:,k-2) +dmu(:,:,:,:,:,Im,:,:,k-2);
266   end
```

Interpolate macro-values to be Dirichlet face values for each patch (Roberts and Kevrekidis 2007; Bunder, Roberts, and Kevrekidis 2017), using the weights pre-computed by `configPatches3()`. Here interpolate to specified order.

For the case where next-to-face values interpolate to the opposite face-values: when we have an ensemble of configurations, different configurations might be coupled to each other, as specified by `patches.le`, `patches.ri`, `patches.to`, `patches.bo`, `patches.fr` and `patches.ba`.

```
282 k=1+patches.EdgyInt; % use centre or two faces
283 u(nx,2:(ny-1),2:(nz-1),:,patches.ri,I,:,:) ...
```

```
284   = U(1,:,:,:,:,:,:,:)*(1-patches.stag) ...
285   +sum( shiftdim(patches.Cwtsr(:,1),-8).*dmu(1,:,:,:,:,:,:,:,:) ,9);
286 u(1 ,2:(ny-1),2:(nz-1),:,patches.le,I,:,:) ...
287   = U(k,:,:,:,:,:,:,:)*(1-patches.stag) ...
288   +sum( shiftdim(patches.Cwtsl(:,1),-8).*dmu(k,:,:,:,:,:,:,:,:) ,9);
```

y-normal face values Interpolate from either the next-to-edge-face values, or the centre-cross-plane values.

```
300   if patches.EdgyInt % interpolate next-to-face values
301     U = u(:,[2 ny-1],2:(nz-1),:,:,I,J,K);
302   else % interpolate centre-cross values
303     U = u(:,j0,2:(nz-1),:,:,I,J,K);
304   end;%if patches.EdgyInt
```

Adjoin extra dimension for the array of differences.

```
310 szUO=size(U); szUO=[szUO ones(1,8-length(szUO)) ordCC];
```

Store finite differences $(\mu\delta, \delta^2, \mu\delta^3, \delta^4, \ldots)$ in this array.

```
317   if ~patches.parallel, dmu = zeros(szUO); % 9D
318   else   dmu = zeros(szUO,patches.codist); % 9D
319   end%if patches.parallel
```

First compute differences $\mu\delta$ and δ^2.

```
325   if patches.stag % use only odd numbered neighbours
326     error('polynomial interpolation not yet for staggered patch coupl
327   else  %disp('starting standard interpolation')
328     dmu(:,:,:,:,:,:,J,:,1) = (U(:,:,:,:,:,:,:,Jp,:) ...
329                               -U(:,:,:,:,:,:,:,Jm,:))/2; %\mu\delta
330     dmu(:,:,:,:,:,:,J,:,2) = (U(:,:,:,:,:,:,:,Jp,:) ...
331        -2*U(:,:,:,:,:,:,:,J,:) +U(:,:,:,:,:,:,:,Jm,:));   %\delta^2
332   end% if stag
```

Recursively take δ^2.

```
338   for k = 3:ordCC
339     dmu(:,:,:,:,:,:,J,:,k) =     dmu(:,:,:,:,:,:,:,Jp,:,k-2) ...
340     -2*dmu(:,:,:,:,:,:,:,J,:,k-2) +dmu(:,:,:,:,:,:,:,Jm,:,k-2);
341   end
```

Interpolate macro-values using the weights pre-computed by `configPatches3()`. An ensemble of configurations may have cross-coupling.

```
k=1+patches.EdgyInt; % use centre or two faces
u(:,ny,2:(nz-1),:,patches.to,:,J,:) ...
  = U(:,1,:,:,:,:,:,:)*(1-patches.stag) ...
  +sum( shiftdim(patches.Cwtsr(:,2),-8).*dmu(:,1,:,:,:,:,:,:,:) ,9);
u(:,1 ,2:(nz-1),:,patches.bo,:,J,:) ...
  = U(:,k,:,:,:,:,:,:)*(1-patches.stag) ...
  +sum( shiftdim(patches.Cwtsl(:,2),-8).*dmu(:,k,:,:,:,:,:,:,:) ,9);
```

z-normal face values Interpolate from either the next-to-edge-face values, or the centre-cross-plane values.

```
  if patches.EdgyInt % interpolate next-to-face values
    U = u(:,:,[2 nz-1],:,:,I,J,K);
  else % interpolate centre-cross values
    U = u(:,:,k0,:,:,I,J,K);
  end;%if patches.EdgyInt
```

Adjoin extra dimension for the array of differences.

```
szUO=size(U); szUO=[szUO ones(1,8-length(szUO)) ordCC];
```

Store finite differences $(\mu\delta, \delta^2, \mu\delta^3, \delta^4, \ldots)$ in this array.

```
  if ~patches.parallel, dmu = zeros(szUO); % 9D
  else   dmu = zeros(szUO,patches.codist); % 9D
  end%if patches.parallel
```

First compute differences $\mu\delta$ and δ^2.

```
  if patches.stag % use only odd numbered neighbours
    error('polynomial interpolation not yet for staggered patch coupl
  else  %disp('starting standard interpolation')
    dmu(:,:,:,:,:,:,:,:,K,1) = (U(:,:,:,:,:,:,:,:,Kp) ...
                              -U(:,:,:,:,:,:,:,:,Km))/2; %\mu\delta
    dmu(:,:,:,:,:,:,:,:,K,2) = (U(:,:,:,:,:,:,:,:,Kp) ...
       -2*U(:,:,:,:,:,:,:,:,K) +U(:,:,:,:,:,:,:,:,Km));   %\delta^2
  end% if stag
```

Recursively take δ^2.

```
404   for k = 3:ordCC
405     dmu(:,:,:,:,:,:,:,K,k) =     dmu(:,:,:,:,:,:,:,:,Kp,k-2) ...
406     -2*dmu(:,:,:,:,:,:,:,:,K,k-2) +dmu(:,:,:,:,:,:,:,:,Km,k-2);
407   end
```

Interpolate macro-values using the weights pre-computed by `configPatches3()`. An ensemble of configurations may have cross-coupling.

```
415 k=1+patches.EdgyInt; % use centre or two faces
416 u(:,:,nz,:,patches.fr,:,:,K) ...
417   = U(:,:,1,:,:,:,:,:,:)*(1-patches.stag) ...
418   +sum( shiftdim(patches.Cwtsr(:,3),-8).*dmu(:,:,1,:,:,:,:,:,:) ,9);
419 u(:,:,1 ,:,patches.ba,:,:,K) ...
420   = U(:,:,k,:,:,:,:,:,:)*(1-patches.stag) ...
421   +sum( shiftdim(patches.Cwtsl(:,3),-8).*dmu(:,:,k,:,:,:,:,:,:) ,9);
```

17.1.2 Case of spectral interpolation

Assumes the domain is macro-periodic.

```
431 else% patches.ordCC<=0, spectral interpolation
```

We interpolate in terms of the patch index, I say, not directly in space. As the macroscale fields are N-periodic in the patch index I, the macroscale Fourier transform writes the centre-patch values as $U_I = \sum_k C_k e^{ik2\pi I/N}$. Then the face-patch values $U_{I\pm r} = \sum_k C_k e^{ik2\pi/N(I\pm r)} = \sum_k C'_k e^{ik2\pi I/N}$ where $C'_k = C_k e^{ikr2\pi/N}$. For N patches we resolve 'wavenumbers' $|k| < N/2$, so set row vector `ks` $= k2\pi/N$ for 'wavenumbers' $k = (0\,, 1\,, \ldots, k_{\max}\,, -k_{\max}\,, \ldots, -1)$ for odd N, and $k = (0\,, 1\,, \ldots, k_{\max}\,, \pm(k_{\max}+1) - k_{\max}\,, \ldots, -1)$ for even N.

Deal with staggered grid by doubling the number of fields and halving the number of patches (`configPatches3` tests there are an even number of patches). Then the patch-ratio is effectively halved. The patch faces are near the middle of the gaps and swapped.

```
454  if patches.stag % transform by doubling the number of fields
455  error('staggered grid not yet implemented??')
456    v=nan(size(u)); % currently to restore the shape of u
457    u=cat(3,u(:,1:2:nPatch,:),u(:,2:2:nPatch,:));
458    stagShift=reshape(0.5*[ones(nVars,1);-ones(nVars,1)],1,1,1,[]);
459    iV=[nVars+1:2*nVars 1:nVars]; % scatter interp to alternate field
460    r=r/2;           % ratio effectively halved
```

```
461     nPatch=nPatch/2; % halve the number of patches
462     nVars=nVars*2;   % double the number of fields
463   else % the values for standard spectral
464      stagShift = 0;
465      iV = 1:nVars;
466   end%if patches.stag
```

Interpolate the three directions in succession, in this way we naturally fill-in face-edge and corner values. Start with x-direction, and give most documentation for that case as the others are essentially the same. Need these indices of patch interior.

```
476 ix = 2:nx-1;   iy = 2:ny-1;   iz = 2:nz-1;
```

x-normal face values Now set wavenumbers into a vector at the correct dimension. In the case of even N these compute the $+$-case for the highest wavenumber zig-zag mode, $k = (0\,, 1\,, \ldots, k_{\max}\,, +(k_{\max}+1) - k_{\max}\,, \ldots, -1)$.

```
489   kMax = floor((Nx-1)/2);
490   kr = shiftdim( rx*2*pi/Nx*(mod((0:Nx-1)+kMax,Nx)-kMax) ,-4);
```

Compute the Fourier transform of the patch values on the centre-planes for all the fields. Unless doing patch-edgy interpolation when FT the next-to-face values. If there are an even number of points, then if complex, treat as positive wavenumber, but if real, treat as cosine. When using an ensemble of configurations, different configurations might be coupled to each other, as specified by `patches.le`, `patches.ri`, `patches.to`, `patches.bo`, `patches.fr` and `patches.ba`.

```
504 if ~patches.EdgyInt
505      Cm = fft( u(i0,iy,iz,:,:,:,:,:) ,[],6);
506      Cp = Cm;
507 else
508      Cm = fft( u(   2,iy,iz ,:,patches.le,:,:,:) ,[],6);
509      Cp = fft( u(nx-1,iy,iz ,:,patches.ri,:,:,:) ,[],6);
510 end%if ~patches.EdgyInt
```

Now invert the Fourier transforms to complete interpolation. Enforce reality when appropriate.

```
517 u(nx,iy,iz,:,:,:,:,:) = uclean( ifft( ...
518     Cm.*exp(1i*(stagShift+kr))  ,[],6) );
```

```
519 u( 1,iy,iz,:,:,:,:,:) = uclean( ifft( ...
520     Cp.*exp(1i*(stagShift-kr))  ,[],6) );
```

y-normal face values Set wavenumbers into a vector.

```
530   kMax = floor((Ny-1)/2);
531   kr = shiftdim( ry*2*pi/Ny*(mod((0:Ny-1)+kMax,Ny)-kMax) ,-5);
```

Compute the Fourier transform of the patch values on the centre-planes for all the fields.

```
538 if ~patches.EdgyInt
539      Cm = fft( u(:,j0,iz,:,:,:,:,:) ,[],7);
540      Cp = Cm;
541 else
542      Cm = fft( u(:,2   ,iz ,:,patches.bo,:,:,:) ,[],7);
543      Cp = fft( u(:,ny-1,iz ,:,patches.to,:,:,:) ,[],7);
544 end%if ~patches.EdgyInt
```

Invert the Fourier transforms to complete interpolation.

```
550 u(:,ny,iz,:,:,:,:,:) = uclean( ifft( ...
551     Cm.*exp(1i*(stagShift+kr))  ,[],7) );
552 u(:, 1,iz,:,:,:,:,:) = uclean( ifft( ...
553     Cp.*exp(1i*(stagShift-kr))  ,[],7) );
```

z-normal face values Set wavenumbers into a vector.

```
563   kMax = floor((Nz-1)/2);
564   kr = shiftdim( rz*2*pi/Nz*(mod((0:Nz-1)+kMax,Nz)-kMax) ,-6);
```

Compute the Fourier transform of the patch values on the centre-planes for all the fields.

```
571 if ~patches.EdgyInt
572      Cm = fft( u(:,:,k0,:,:,:,:,:) ,[],8);
573      Cp = Cm;
574 else
575      Cm = fft( u(:,:,2    ,:,patches.ba,:,:,:) ,[],8);
576      Cp = fft( u(:,:,nz-1 ,:,patches.fr,:,:,:) ,[],8);
577 end%if ~patches.EdgyInt
```

Invert the Fourier transforms to complete interpolation.

```
u(:,:,nz,:,:,:,:,:) = uclean( ifft( ...
    Cm.*exp(1i*(stagShift+kr))  ,[],8) );
u(:,:, 1,:,:,:,:,:) = uclean( ifft( ...
    Cp.*exp(1i*(stagShift-kr))  ,[],8) );

end% if ordCC>0
```

17.2 Non-periodic macroscale interpolation

```
else% patches.periodic false
assert(~patches.stag, ...
'not yet implemented staggered grids for non-periodic')
```

Determine the order of interpolation `px`, `py` and `pz` (potentially different in the different directions!), and hence size of the (forward) divided difference tables in `F` (9D) for interpolating to left/right, top/bottom, and front/back faces. Because of the product-form of the patch grid, and because we are doing *only* either edgy interpolation or cross-patch interpolation (*not* just the centre patch value), the interpolations are all 1D interpolations.

```
if patches.ordCC<1
     px = Nx-1;  py = Ny-1;  pz = Nz-1;
else px = min(patches.ordCC,Nx-1);
     py = min(patches.ordCC,Ny-1);
     pz = min(patches.ordCC,Nz-1);
end
% interior indices of faces  (ix n/a)
ix=2:nx-1;  iy=2:ny-1;  iz=2:nz-1;
```

17.2.1 x-direction values

Set function values in first 'column' of the tables for every variable and across ensemble. For `EdgyInt`, the 'reversal' of the next-to-face values are because their values are to interpolate to the opposite face of each patch. [28]

```
  F = nan(patches.EdgyInt+1,ny-2,nz-2,nVars,nEnsem,Nx,Ny,Nz,px+1);
  if patches.EdgyInt % interpolate next-to-face values
```

[28] **ToDo:** Have no plans to implement core averaging as yet.

```
641       F(:,:,:,:,:,:,:,:,1) = u([nx-1 2],iy,iz,:,:,:,:,:);
642       X = patches.x([nx-1 2],:,:,:,:,:,:,:);
643     else % interpolate mid-patch cross-patch values
644       F(:,:,:,:,:,:,:,:,1) = u(i0,iy,iz,:,:,:,:,:);
645       X = patches.x(i0,:,:,:,:,:,:,:);
646     end%if patches.EdgyInt
```

Form tables of divided differences Compute tables of (forward) divided differences (e.g., Wikipedia 2022) for every variable, and across ensemble, and in both directions, and for all three types of faces (left/right, top/bottom, and front/back). Recursively find all divided differences in the respective direction.

```
659 for q = 1:px
660   i = 1:Nx-q;
661   F(:,:,:,:,:,i,:,:,q+1) ...
662   = ( F(:,:,:,:,:,:,i+1,:,:,q)-F(:,:,:,:,:,:,i,:,:,q)) ...
663    ./(X(:,:,:,:,:,:,i+q,:,:)  -X(:,:,:,:,:,:,i,:,:));
664 end
```

Interpolate with divided differences Now interpolate to find the face-values on left/right faces at `Xface` for every interior `Y,Z`.

```
673 Xface = patches.x([1 nx],:,:,:,:,:,:,:);
```

Code Horner's recursive evaluation of the interpolation polynomials. Indices `i` are those of the left face of each interpolation stencil, because the table is of forward differences. This alternative: the case of order p_x, p_y and p_z interpolation across the domain, asymmetric near the boundaries of the rectangular domain.

```
684   i = max(1,min(1:Nx,Nx-ceil(px/2))-floor(px/2));
685   Uface = F(:,:,:,:,:,i,:,:,px+1);
686   for q = px:-1:1
687     Uface = F(:,:,:,:,:,i,:,:,q) ...
688     +(Xface-X(:,:,:,:,:,i+q-1,:,:)).*Uface;
689   end
```

Finally, insert face values into the array of field values, using the required ensemble shifts.

```
697 u(1 ,iy,iz,:,patches.le,:,:,:) = Uface(1,:,:,:,:,:,:,:);
698 u(nx,iy,iz,:,patches.ri,:,:,:) = Uface(2,:,:,:,:,:,:,:);
```

17.2.2 y-direction values

Set function values in first 'column' of the tables for every variable and across ensemble.

```
708   F = nan(nx,patches.EdgyInt+1,nz-2,nVars,nEnsem,Nx,Ny,Nz,py+1);
709   if patches.EdgyInt % interpolate next-to-face values
710     F(:,:,:,:,:,:,:,:,1) = u(:,[ny-1 2],iz,:,:,:,:,:);
711     Y = patches.y(:,[ny-1 2],:,:,:,:,:,:);
712   else % interpolate mid-patch cross-patch values
713     F(:,:,:,:,:,:,:,:,1) = u(:,j0,iz,:,:,:,:,:);
714     Y = patches.y(:,j0,:,:,:,:,:,:);
715   end%if patches.EdgyInt
```

Form tables of divided differences.

```
721 for q = 1:py
722   j = 1:Ny-q;
723   F(:,:,:,:,:,:,j,:,q+1) ...
724   = ( F(:,:,:,:,:,:,j+1,:,q)-F(:,:,:,:,:,:,j,:,q)) ...
725    ./(Y(:,:,:,:,:,:,j+q,:)  -Y(:,:,:,:,:,:,j,:));
726 end
```

Interpolate to find the top/bottom faces `Yface` for every x and interior z.

```
733 Yface = patches.y(:,[1 ny],:,:,:,:,:,:);
```

Code Horner's recursive evaluation of the interpolation polynomials. Indices `j` are those of the bottom face of each interpolation stencil, because the table is of forward differences.

```
742   j = max(1,min(1:Ny,Ny-ceil(py/2))-floor(py/2));
743   Uface = F(:,:,:,:,:,:,j,:,py+1);
744   for q = py:-1:1
745     Uface = F(:,:,:,:,:,:,j,:,q) ...
746     +(Yface-Y(:,:,:,:,:,:,j+q-1,:)).*Uface;
747   end
```

Finally, insert face values into the array of field values, using the required ensemble shifts.

```
755 u(:,1 ,iz,:,patches.bo,:,:,:) = Uface(:,1,:,:,:,:,:,:);
756 u(:,ny,iz,:,patches.to,:,:,:) = Uface(:,2,:,:,:,:,:,:);
```

17.2.3 z-direction values

Set function values in first 'column' of the tables for every variable and across ensemble.

```
766   F = nan(nx,ny,patches.EdgyInt+1,nVars,nEnsem,Nx,Ny,Nz,pz+1);
767   if patches.EdgyInt % interpolate next-to-face values
768     F(:,:,:,:,:,:,:,:,1) = u(:,:,[nz-1 2],:,:,:,:,:);
769     Z = patches.z(:,:,[nz-1 2],:,:,:,:,:);
770   else % interpolate mid-patch cross-patch values
771     F(:,:,:,:,:,:,:,:,1) = u(:,:,k0,:,:,:,:,:);
772     Z = patches.z(:,:,k0,:,:,:,:,:);
773   end%if patches.EdgyInt
```

Form tables of divided differences.

```
779 for q = 1:pz
780   k = 1:Nz-q;
781   F(:,:,:,:,:,:,:,k,q+1) ...
782   = ( F(:,:,:,:,:,:,:,k+1,q)-F(:,:,:,:,:,:,:,k,q)) ...
783    ./(Z(:,:,:,:,:,:,:,k+q)  -Z(:,:,:,:,:,:,:,k));
784 end
```

Interpolate to find the face-values on front/back faces `Zface` for every x, y.

```
791 Zface = patches.z(:,:,[1 nz],:,:,:,:,:);
```

Code Horner's recursive evaluation of the interpolation polynomials. Indices `k` are those of the bottom face of each interpolation stencil, because the table is of forward differences.

```
800   k = max(1,min(1:Nz,Nz-ceil(pz/2))-floor(pz/2));
801   Uface = F(:,:,:,:,:,:,:,k,pz+1);
802   for q = pz:-1:1
803     Uface = F(:,:,:,:,:,:,:,k,q) ...
804     +(Zface-Z(:,:,:,:,:,:,:,k+q-1)).*Uface;
805   end
```

Finally, insert face values into the array of field values, using the required ensemble shifts.

```
813 u(:,:,1 ,:,patches.fr,:,:,:) = Uface(:,:,1,:,:,:,:,:);
814 u(:,:,nz,:,patches.ba,:,:,:) = Uface(:,:,2,:,:,:,:,:);
```

17.2.4 Optional NaNs for safety

We want a user to set outer face values on the extreme patches according to the microscale boundary conditions that hold at the extremes of the domain. Consequently, override their computed interpolation values with `NaN`.

```
826 u( 1,:,:,:,:, 1,:,:) = nan;
827 u(nx,:,:,:,:,Nx,:,:) = nan;
828 u(:, 1,:,:,:,:, 1,:) = nan;
829 u(:,ny,:,:,:,:,Ny,:) = nan;
830 u(:,:, 1,:,:,:,:, 1) = nan;
831 u(:,:,nz,:,:,:,:,Nz) = nan;
```

End of the non-periodic interpolation code.

```
838 end%if patches.periodic else
```

Fin, returning the 8D array of field values with interpolated faces.

```
849 end% function patchEdgeInt3
```

18 `configPatches3()`: configures spatial patches in 3D

Makes the struct `patches` for use by the patch/gap-tooth time derivative/step function `patchSys3()`, and possibly other patch functions. Section 18.1 and **??** list examples of its use.

```
20 function patches = configPatches3(fun,Xlim,Dom ...
21     ,nPatch,ordCC,dx,nSubP,varargin)
```

Input If invoked with no input arguments, then executes an example of simulating a heterogeneous wave PDE—see Section 18.1 for an example code.

- `fun` is the name of the user function, `fun(t,u,patches)` or `fun(t,u)`, that computes time-derivatives (or time-steps) of quantities on the 3D micro-grid within all the 3D patches.
- `Xlim` array/vector giving the rectangular-cuboid macro-space domain of the computation: namely $[\texttt{Xlim(1)}, \texttt{Xlim(2)}] \times [\texttt{Xlim(3)}, \texttt{Xlim(4)} \times [\texttt{Xlim(5)}, \texttt{Xlim(6)}]$. If `Xlim` has two elements, then the domain is the cubic domain of the same interval in all three directions.

- `Dom` sets the type of macroscale conditions for the patches, and reflects the type of microscale boundary conditions of the problem. If `Dom` is `NaN` or `[]`, then the field `u` is triply macro-periodic in the 3D spatial domain, and resolved on equi-spaced patches. If `Dom` is a character string, then that specifies the `.type` of the following structure, with `.bcOffset` set to the default zero. Otherwise `Dom` is a structure with the following components.

  - `.type`, string, of either `'periodic'` (the default), `'equispace'`, `'chebyshev'`, `'usergiven'`. For all cases except `'periodic'`, users *must* code into `fun` the micro-grid boundary conditions that apply at the left/right/bottom/top/back/front faces of the leftmost/rightmost/bottommost/topmost/backmost/frontmost patches, respectively.
  - `.bcOffset`, optional one, three or six element vector/array, in the cases of `'equispace'` or `'chebyshev'` the patches are placed so the left/right macroscale boundaries are aligned to the left/right faces of the corresponding extreme patches, but offset by `bcOffset` of the sub-patch micro-grid spacing. For example, use `bcOffset=0` when the micro-code applies Dirichlet boundary values on the extreme face micro-grid points, whereas use `bcOffset=0.5` when the microcode applies Neumann boundary conditions halfway between the extreme face micro-grid points. Similarly for the top, bottom, back, and front faces.

    If `.bcOffset` is a scalar, then apply the same offset to all boundaries. If three elements, then apply the first offset to both x-boundaries, the second offset to both y-boundaries, and the third offset to both z-boundaries. If six elements, then apply the first two offsets to the respective x-boundaries, the middle two offsets to the respective y-boundaries, and the last two offsets to the respective z-boundaries.
  - `.X`, optional vector/array with `nPatch(1)` elements, in the case `'usergiven'` it specifies the x-locations of the centres of the patches—the user is responsible the locations makes sense.
  - `.Y`, optional vector/array with `nPatch(2)` elements, in the case `'usergiven'` it specifies the y-locations of the centres of the patches—the user is responsible the locations makes sense.
  - `.Z`, optional vector/array with `nPatch(3)` elements, in the case `'usergiven'` it specifies the z-locations of the centres of the patches—

the user is responsible the locations makes sense.

- `nPatch` sets the number of equi-spaced spatial patches: if scalar, then use the same number of patches in all three directions, otherwise `nPatch(1:3)` gives the number (≥ 1) of patches in each direction.

- `ordCC` is the 'order' of interpolation for inter-patch coupling across empty space of the macroscale patch values to the face-values of the patches: currently must be $0, 2, 4, \ldots$; where 0 gives spectral interpolation.

- `dx` (real—scalar or three elements) is usually the sub-patch micro-grid spacing in x, y and z. If scalar, then use the same `dx` in all three directions, otherwise `dx(1:3)` gives the spacing in each of the three directions.

  However, if `Dom` is `NaN` (as for pre-2023), then `dx` actually is `ratio` (scalar or three elements), namely the ratio of (depending upon `EdgyInt`) either the half-width or full-width of a patch to the equi-spacing of the patch mid-points. So either `ratio` $= \frac{1}{2}$ means the patches abut and `ratio` $= 1$ is overlapping patches as in holistic discretisation, or `ratio` $= 1$ means the patches abut. Small `ratio` should greatly reduce computational time.

- `nSubP` is the number of equi-spaced microscale lattice points in each patch: if scalar, then use the same number in all three directions, otherwise `nSubP(1:3)` gives the number in each direction. If not using `EdgyInt`, then must be odd so that there is/are centre-patch micro-grid point/planes in each patch.

- `'nEdge'` (not yet implemented), *optional*, default=1, for each patch, the number of face values set by interpolation at the face regions of each patch. The default is one (suitable for microscale lattices with only nearest neighbour interactions).

- `'EdgyInt'`, true/false, *optional*, default=false. If true, then interpolate to left/right/top/bottom/front/back face-values from right/left/bottom/top/back/front next-to-face values. If false or omitted, then interpolate from centre-patch planes.

- `'nEnsem'`, *optional-experimental*, default one, but if more, then an ensemble over this number of realisations.

- `'hetCoeffs'`, *optional*, default empty. Supply a 3D or 4D array of microscale heterogeneous coefficients to be used by the given microscale

`fun` in each patch. Say the given array `cs` is of size $m_x \times m_y \times m_z \times n_c$, where n_c is the number of different arrays of coefficients. For example, in heterogeneous diffusion, $n_c = 3$ for the diffusivities in the *three* different spatial directions (or $n_c = 6$ for the diffusivity tensor). The coefficients are to be the same for each and every patch. However, macroscale variations are catered for by the n_c coefficients being n_c parameters in some macroscale formula.

  - If `nEnsem` $= 1$, then the array of coefficients is just tiled across the patch size to fill up each patch, starting from the $(1, 1, 1)$-point in each patch.
  - If `nEnsem` > 1 (value immaterial), then reset `nEnsem` $:= m_x \cdot m_y \cdot m_z$ and construct an ensemble of all $m_x \cdot m_y \cdot m_z$ phase-shifts of the coefficients. In this scenario, the inter-patch coupling couples different members in the ensemble. When `EdgyInt` is true, and when the coefficients are diffusivities/elasticities in x, y, z-directions, respectively, then this coupling cunningly preserves symmetry.

- `'parallel'`, true/false, *optional*, default=false. If false, then all patch computations are on the user's main CPU—although a user may well separately invoke, say, a GPU to accelerate sub-patch computations.

  If true, and it requires that you have MATLAB's Parallel Computing Toolbox, then it will distribute the patches over multiple CPUs/cores. In MATLAB, only one array dimension can be split in the distribution, so it chooses the one space dimension x, y, z corresponding to the highest `nPatch` (if a tie, then chooses the rightmost of x, y, z). A user may correspondingly distribute arrays with property `patches.codist`, or simply use formulas invoking the preset distributed arrays `patches.x`, `patches.y`, and `patches.z`. If a user has not yet established a parallel pool, then a 'local' pool is started.

Output The struct `patches` is created and set with the following components. If no output variable is provided for `patches`, then make the struct available as a global variable.[29]

```
217 if nargout==0, global patches, end
```

[29] When using `spmd` parallel computing, it is generally best to avoid global variables, and so instead prefer using an explicit output variable.

- `.fun` is the name of the user's function `fun(t,u,patches)` or `fun(t,u)` that computes the time derivatives (or steps) on the patchy lattice.
- `.ordCC` is the specified order of inter-patch coupling.
- `.periodic`: either true, for interpolation on the macro-periodic domain; or false, for general interpolation by divided differences over non-periodic domain or unevenly distributed patches.
- `.stag` is true for interpolation using only odd neighbouring patches as for staggered grids, and false for the usual case of all neighbour coupling—not yet implemented.
- `.Cwtsr` and `.Cwtsl` are the `ordCC` $\times$ 3-array of weights for the inter-patch interpolation onto the right/top/front and left/bottom/back faces (respectively) with patch:macroscale ratio as specified or as derived from `dx`.
- `.x` (8D) is `nSubP(1)` $\times 1 \times 1 \times 1 \times 1 \times$ `nPatch(1)` $\times 1 \times 1$ array of the regular spatial locations x_{iI} of the microscale grid points in every patch.
- `.y` (8D) is $1 \times$ `nSubP(2)` $\times 1 \times 1 \times 1 \times 1 \times$ `nPatch(2)` $\times 1$ array of the regular spatial locations y_{jJ} of the microscale grid points in every patch.
- `.z` (8D) is $1 \times 1 \times$ `nSubP(3)` $\times 1 \times 1 \times 1 \times 1 \times$ `nPatch(3)` array of the regular spatial locations z_{kK} of the microscale grid points in every patch.
- `.ratio` 1×3, only for macro-periodic conditions, are the size ratios of every patch.
- `.nEdge` is, for each patch, the number of face values set by interpolation at the face regions of each patch.
- `.le`, `.ri`, `.bo`, `.to`, `.ba`, `.fr` determine inter-patch coupling of members in an ensemble. Each a column vector of length `nEnsem`.
- `.cs` either
  - `[]` 0D, or
  - if `nEnsem` $= 1$, (`nSubP(1)` $-1) \times$ (`nSubP(2)` $-1) \times$ (`nSubP(3)` $-1) \times n_c$ 4D array of microscale heterogeneous coefficients, or

– if `nEnsem` > 1, (`nSubP(1)` $-1) \times$ (`nSubP(2)` $-1) \times$ (`nSubP(3)` $-1) \times$ $n_c \times m_x m_y m_z$ 5D array of $m_x m_y m_z$ ensemble of phase-shifts of the microscale heterogeneous coefficients.

- `.parallel`, logical: true if patches are distributed over multiple CPUs/ cores for the Parallel Computing Toolbox, otherwise false (the default is to activate the *local* pool).

- `.codist`, *optional*, describes the particular parallel distribution of arrays over the active parallel pool.

18.1 If no arguments, then execute an example

```
305 if nargin==0
306 disp('With no arguments, simulate example of heterogeneous wave')
```

The code here shows one way to get started: a user's script may have the following three steps ("$\mapsto$" denotes function recursion).

1. configPatches3
2. ode23 integrator $\mapsto$ patchSys3 $\mapsto$ user's PDE
3. process results

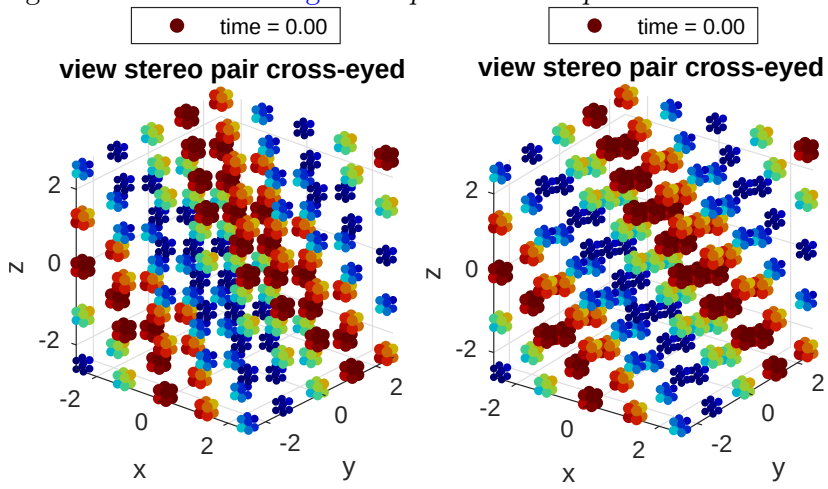
Set random heterogeneous coefficients of period two in each of the three directions. Crudely normalise by the harmonic mean so the macro-wave time scale is roughly one.

```
324 mPeriod = [2 2 2];
325 cHetr = exp(0.9*randn([mPeriod 3]));
326 cHetr = cHetr*mean(1./cHetr(:))
```

Establish global patch data struct to interface with a function coding a nonlinear 'diffusion' PDE: to be solved on $[-\pi, \pi]^3$-periodic domain, with 5^3 patches, spectral interpolation (0) couples the patches, each patch with micro-grid spacing 0.22 (relatively large for visualisation), and with 4^3 points forming each patch.

```
338 global patches
339 patches = configPatches3(@heteroWave3,[-pi pi], 'periodic' ...
340     , 5, 0, 0.22, mPeriod+2 ,'EdgyInt',true ...
341     ,'hetCoeffs',cHetr);
```

Figure 17: initial field $u(x, y, z, t)$ at time $t = 0$ of the patch scheme applied to a heterogeneous wave PDE*: Figure 18 plots the computed field at time $t = 6$.*



Set a wave initial state using auto-replication of the spatial grid, and as Figure 17 shows. This wave propagates diagonally across space. Concatenate the two u, v-fields to be the two components of the fourth dimension.

```
u0 = 0.5+0.5*sin(patches.x+patches.y+patches.z);
v0 =    -0.5*cos(patches.x+patches.y+patches.z)*sqrt(3);
uv0 = cat(4,u0,v0);
```

Integrate in time to $t = 6$ using standard functions. In Matlab `ode15s` would be natural as the patch scheme is naturally stiff, but `ode23` is much quicker (Maclean, Bunder, and Roberts 2021, Fig. 4).

```
disp('Simulate heterogeneous wave u_tt=div[C*grad(u)]')
if ~exist('OCTAVE_VERSION','builtin')
    [ts,us] = ode23(@patchSys3,linspace(0,6),uv0(:));
else %disp('octave version is very slow for me')
    lsode_options('absolute tolerance',1e-4);
    lsode_options('relative tolerance',1e-4);
    [ts,us] = odeOcts(@patchSys3,[0 1 2],uv0(:));
end
```

Animate the computed simulation to end with Figure 18. Use `patchEdgeInt3` to obtain patch-face values in order to most easily reconstruct the array data structure.

Replicate x, y, and z arrays to get individual spatial coordinates of every data point. Then, optionally, set faces to `nan` so the plot just shows patch-interior data.

```
figure(1), clf, colormap(0.8*jet)
xs = patches.x+0*patches.y+0*patches.z;
ys = patches.y+0*patches.x+0*patches.z;
zs = patches.z+0*patches.y+0*patches.x;
if 1, xs([1 end],:,:,:)=nan;
      xs(:,[1 end],:,:)=nan;
      xs(:,:,[1 end],:)=nan;
end;%option
j=find(~isnan(xs));
```

In the scatter plot, these functions `pix()` and `col()` map the u-data values to the size of the dots and to the colour of the dots, respectively.

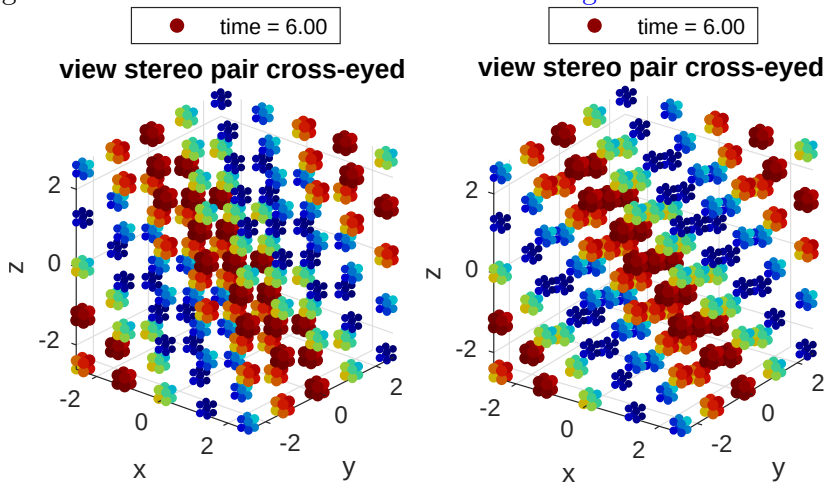
```
pix = @(u) 15*abs(u)+7;
col = @(u) sign(u).*abs(u);
```

Loop to plot at each and every time step.

```
for i = 1:length(ts)
  uv = patchEdgeInt3(us(i,:));
  u = uv(:,:,:,1,:);
  for p=1:2
    subplot(1,2,p)
    if (i==1)| exist('OCTAVE_VERSION','builtin')
      scat(p) = scatter3(xs(j),ys(j),zs(j),'filled');
      axis equal, caxis(col([0 1])), view(45-5*p,25)
      xlabel('x'), ylabel('y'), zlabel('z')
      title('view stereo pair cross-eyed')
    end % in matlab just update values
    set(scat(p),'CData',col(u(j)) ...
       ,'SizeData',pix((8+xs(j)-ys(j)+zs(j))/6+0*u(j)));
    legend(['time = ' num2str(ts(i),'%4.2f')],'Location','north')
  end
```

Optionally save the initial condition to graphic file for Figure 15, and optionally save the last plot.

Figure 18: field $u(x, y, z, t)$ at time $t = 6$ of the patch scheme applied to the heterogeneous wave PDE *with initial condition in Figure 17.*




```
  if i==1,
    ifOurCf2eps([mfilename 'ic'])
    disp('Type space character to animate simulation')
    pause
  else pause(0.05)
  end
end% i-loop over all times
ifOurCf2eps([mfilename 'fin'])
```

Upon finishing execution of the example, exit this function.

```
return
end%if no arguments
```

18.2 Parse input arguments and defaults

```
p = inputParser;
fnValidation = @(f) isa(f, 'function_handle'); %test for fn name
addRequired(p,'fun',fnValidation);
addRequired(p,'Xlim',@isnumeric);
%addRequired(p,'Dom'); % too flexible
addRequired(p,'nPatch',@isnumeric);
addRequired(p,'ordCC',@isnumeric);
```

```
addRequired(p,'dx',@isnumeric);
addRequired(p,'nSubP',@isnumeric);
addParameter(p,'nEdge',1,@isnumeric);
addParameter(p,'EdgyInt',false,@islogical);
addParameter(p,'nEnsem',1,@isnumeric);
addParameter(p,'hetCoeffs',[],@isnumeric);
addParameter(p,'parallel',false,@islogical);
%addParameter(p,'nCore',1,@isnumeric); % not yet implemented
parse(p,fun,Xlim,nPatch,ordCC,dx,nSubP,varargin{:});
```

Set the optional parameters.

```
patches.nEdge = p.Results.nEdge;
patches.EdgyInt = p.Results.EdgyInt;
patches.nEnsem = p.Results.nEnsem;
cs = p.Results.hetCoeffs;
patches.parallel = p.Results.parallel;
%patches.nCore = p.Results.nCore;
```

Initially duplicate parameters for three space dimensions as needed.

```
if numel(Xlim)==2,   Xlim = repmat(Xlim,1,3); end
if numel(nPatch)==1, nPatch = repmat(nPatch,1,3); end
if numel(dx)==1,     dx = repmat(dx,1,3); end
if numel(nSubP)==1,  nSubP = repmat(nSubP,1,3); end
```

Check parameters.

```
assert(Xlim(1)<Xlim(2) ...
      ,'first pair of Xlim must be ordered increasing')
assert(Xlim(3)<Xlim(4) ...
      ,'second pair of Xlim must be ordered increasing')
assert(Xlim(5)<Xlim(6) ...
      ,'third pair of Xlim must be ordered increasing')
assert(patches.nEdge==1 ...
      ,'multi-edge-value interp not yet implemented')
assert(all(2*patches.nEdge<nSubP) ...
      ,'too many edge values requested')
%if patches.nCore>1
%    warning('nCore>1 not yet tested in this version')
%    end
```

For compatibility with pre-2023 functions, if parameter `Dom` is `Nan`, then we set the `ratio` to be the value of the so-called `dx` vector.

```
if ~isstruct(Dom), pre2023=isnan(Dom);
else pre2023=false; end
if pre2023, ratio=dx; dx=nan; end
```

Default macroscale conditions are periodic with evenly spaced patches.

```
if isempty(Dom), Dom=struct('type','periodic'); end
if (~isstruct(Dom))&isnan(Dom), Dom=struct('type','periodic'); end
```

If `Dom` is a string, then just set type to that string, and subsequently set corresponding defaults for others fields.

```
if ischar(Dom), Dom=struct('type',Dom); end
```

We allow different macroscale domain conditions in the different directions. But for the moment do not allow periodic to be mixed with the others (as the interpolation mechanism is different code)—hence why we choose `periodic` be seven characters, whereas the others are eight characters. The different conditions are coded in different rows of `Dom.type`, so we duplicate the string if only one row specified.

```
if size(Dom.type,1)==1, Dom.type=repmat(Dom.type,3,1); end
```

Check what is and is not specified, and provide default of Dirichlet boundaries if no `bcOffset` specified when needed. Do so for all three directions independently.

```
patches.periodic=false;
for p=1:3
switch Dom.type(p,:)
case 'periodic'
    patches.periodic=true;
    if isfield(Dom,'bcOffset')
    warning('bcOffset not available for Dom.type = periodic'), end
    msg=' not available for Dom.type = periodic';
    if isfield(Dom,'X'), warning(['X' msg]), end
    if isfield(Dom,'Y'), warning(['Y' msg]), end
    if isfield(Dom,'Z'), warning(['Z' msg]), end
case {'equispace','chebyshev'}
```

```
    if ~isfield(Dom,'bcOffset'), Dom.bcOffset=zeros(2,3); end
    % for mixed with usergiven, following should still work
    if numel(Dom.bcOffset)==1
        Dom.bcOffset=repmat(Dom.bcOffset,2,3); end
    if numel(Dom.bcOffset)==3
        Dom.bcOffset=repmat(Dom.bcOffset(:)',2,1); end
    msg=' not available for Dom.type = equispace or chebyshev';
    if (p==1)& isfield(Dom,'X'), warning(['X' msg]), end
    if (p==2)& isfield(Dom,'Y'), warning(['Y' msg]), end
    if (p==3)& isfield(Dom,'Z'), warning(['Z' msg]), end
case 'usergiven'
%    if isfield(Dom,'bcOffset')
%    warning('bcOffset not available for usergiven Dom.type'), end
    msg=' required for Dom.type = usergiven';
    if p==1, assert(isfield(Dom,'X'),['X' msg]), end
    if p==2, assert(isfield(Dom,'Y'),['Y' msg]), end
    if p==3, assert(isfield(Dom,'Z'),['Z' msg]), end
otherwise
    error([Dom.type 'is unknown Dom.type'])
end%switch Dom.type
end%for p
```

18.3 The code to make patches

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. Spectral coupling is `ordCC` of 0 or (not yet??) -1.

```
assert((ordCC>=-1) & (floor(ordCC)==ordCC), ...
    'ordCC out of allowed range integer>=-1')
```

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

```
patches.stag = mod(ordCC,2);
assert(patches.stag==0,'staggered not yet implemented??')
ordCC = ordCC+patches.stag;
patches.ordCC = ordCC;
```

Check for staggered grid and periodic case.

```
656 if patches.stag, assert(all(mod(nPatch,2)==0), ...
657     'Require an even number of patches for staggered grid')
658 end
```

Set the macro-distribution of patches Third, set the centre of the patches in the macroscale grid of patches. Loop over the coordinate directions, setting the distribution into `Q` and finally assigning to array of corresponding direction.

```
673 for q=1:3
674 qq=2*q-1;
```

Distribution depends upon `Dom.type`:

```
680 switch Dom.type(q,:)
```

The periodic case is evenly spaced within the spatial domain. Store the size ratio in `patches`.

```
688 case 'periodic'
689   Q=linspace(Xlim(qq),Xlim(qq+1),nPatch(q)+1);
690   DQ=Q(2)-Q(1);
691   Q=Q(1:nPatch(q))+diff(Q)/2;
692   pEI=patches.EdgyInt;% abbreviation
693   if pre2023, dx(q) = ratio(q)*DQ/(nSubP(q)-1-pEI)*(2-pEI);
694   else        ratio(q) = dx(q)/DQ*(nSubP(q)-1-pEI)/(2-pEI);
695   end
696   patches.ratio=ratio;
```

The equi-spaced case is also evenly spaced but with the extreme edges aligned with the spatial domain boundaries, modified by the offset.

```
705 case 'equispace'
706   Q=linspace(Xlim(qq)+((nSubP(q)-1)/2-Dom.bcOffset(qq))*dx(q) ...
707           ,Xlim(qq+1)-((nSubP(q)-1)/2-Dom.bcOffset(qq+1))*dx(q) ...
708           ,nPatch(q));
709   DQ=diff(Q(1:2));
710   width=(1+patches.EdgyInt)/2*(nSubP(q)-1-patches.EdgyInt)*dx;
711   if DQ<width*0.999999
712      warning('too many equispace patches (double overlapping)')
713      end
```

The Chebyshev case is spaced according to the Chebyshev distribution in order to reduce macro-interpolation errors, $Q_i \propto -\cos(i\pi/N)$, but with the extreme edges aligned with the spatial domain boundaries, modified by the offset, and modified by possible 'boundary layers'. [30]

```
case 'chebyshev'
  halfWidth=dx(q)*(nSubP(q)-1)/2;
  Q1 = Xlim(1)+halfWidth-Dom.bcOffset(qq)*dx(q);
  Q2 = Xlim(2)-halfWidth+Dom.bcOffset(qq+1)*dx(q);
%  Q = (Q1+Q2)/2-(Q2-Q1)/2*cos(linspace(0,pi,nPatch));
```

Search for total width of 'boundary layers' so that in the interior the patches are non-overlapping Chebyshev. But the width for assessing overlap of patches is the following variable `width`.

```
  width=(1+patches.EdgyInt)/2*(nSubP(q)-1-patches.EdgyInt)*dx(q);
  for b=0:2:nPatch(q)-2
    DQmin=(Q2-Q1-b*width)/2*( 1-cos(pi/(nPatch(q)-b-1)) );
    if DQmin>width, break, end
  end%for
  if DQmin<width*0.999999
    warning('too many Chebyshev patches (mid-domain overlap)')
  end%if
```

Assign the centre-patch coordinates.

```
  Q =[ Q1+(0:b/2-1)*width ...
       (Q1+Q2)/2-(Q2-Q1-b*width)/2*cos(linspace(0,pi,nPatch(q)-b)) ..
       Q2+(1-b/2:0)*width ];
```

The user-given case is entirely up to a user to specify, we just ensure it has the correct shape of a row.

```
case 'usergiven'
  if q==1, Q = reshape(Dom.X,1,[]); end
  if q==2, Q = reshape(Dom.Y,1,[]); end
  if q==3, Q = reshape(Dom.Z,1,[]); end
end%switch Dom.type
```

[30] However, maybe overlapping patches near a boundary should be viewed as some sort of spatially analogue of the 'christmas tree' of projective integration and its integration to a slow manifold. Here maybe the overlapping patches allow for a 'christmas tree' approach to the boundary layers. Needs to be explored??

Assign Q-coordinates to the correct spatial direction. At this stage they are all rows.

```
778 if q==1, X=Q; end
779 if q==2, Y=Q; end
780 if q==3, Z=Q; end
781 end%for q
```

Construct the micro-grids Construct the microscale in each patch. Reshape the grid to be 8D to suit dimensions (micro,Vars,Ens,macro).

```
796 nSubP = reshape(nSubP,1,3); % force to be row vector
797 assert(patches.EdgyInt | all(mod(nSubP,2)==1), ...
798     'configPatches3: nSubP must be odd')
799 i0 = (nSubP(1)+1)/2;
800 patches.x = reshape( dx(1)*(-i0+1:i0-1)'+X ...
801                     ,nSubP(1),1,1,1,1,nPatch(1),1,1);
802 i0 = (nSubP(2)+1)/2;
803 patches.y = reshape( dx(2)*(-i0+1:i0-1)'+Y ...
804                     ,1,nSubP(2),1,1,1,1,nPatch(2),1);
805 i0 = (nSubP(3)+1)/2;
806 patches.z = reshape( dx(3)*(-i0+1:i0-1)'+Z ...
807                     ,1,1,nSubP(3),1,1,1,1,nPatch(3));
```

Pre-compute weights for macro-periodic In the case of macro-periodicity, precompute the weightings to interpolate field values for coupling. [31]

```
819 if patches.periodic
820   ratio = reshape(ratio,1,3); % force to be row vector
821   patches.ratio = ratio;
822   if ordCC>0
823       [Cwtsr,Cwtsl] = patchCwts(ratio,ordCC,patches.stag);
824       patches.Cwtsr = Cwtsr;  patches.Cwtsl = Cwtsl;
825   end%if
826 end%if patches.periodic
```

18.4 Set ensemble inter-patch communication

For `EdgyInt` or centre interpolation respectively,

[31] **ToDo:** Might sometime extend to coupling via derivative values.

- the right-face/centre realisations `1:nEnsem` are to interpolate to left-face `le`, and
- the left-face/centre realisations `1:nEnsem` are to interpolate to `re`.

`re` and `li` are 'transposes' of each other as `re(li)=le(ri)` are both `1:nEnsem`. Similarly for bottom-face/centre interpolation to top-face via `to`, top-face/centre interpolation to bottom-face via `bo`, back-face/centre interpolation to front-face via `fr`, and front-face/centre interpolation to back-face via `ba`.

The default is nothing shifty. This setting reduces the number of if-statements in function `patchEdgeInt3()`.

```
855 nE = patches.nEnsem;
856 patches.le = 1:nE;  patches.ri = 1:nE;
857 patches.bo = 1:nE;  patches.to = 1:nE;
858 patches.ba = 1:nE;  patches.fr = 1:nE;
```

However, if heterogeneous coefficients are supplied via `hetCoeffs`, then do some non-trivial replications. First, get microscale periods, patch size, and replicate many times in order to subsequently sub-sample: `nSubP` times should be enough. If `cs` is more then 4D, then the higher-dimensions are reshaped into the 4th dimension.

```
870 if ~isempty(cs)
871   [mx,my,mz,nc] = size(cs);
872   nx = nSubP(1); ny = nSubP(2); nz = nSubP(3);
873   cs = repmat(cs,nSubP);
```

If only one member of the ensemble is required, then sub-sample to patch size, and store coefficients in `patches` as is.

```
881   if nE==1, patches.cs = cs(1:nx-1,1:ny-1,1:nz-1,:); else
```

But for `nEnsem` > 1 an ensemble of $m_x m_y m_z$ phase-shifts of the coefficients is constructed from the over-supply. Here code phase-shifts over the periods—the phase shifts are like Hankel-matrices.

```
891     patches.nEnsem = mx*my*mz;
892     patches.cs = nan(nx-1,ny-1,nz-1,nc,mx,my,mz);
893     for k = 1:mz
894       ks = (k:k+nz-2);
895       for j = 1:my
```

```
896           js = (j:j+ny-2);
897           for i = 1:mx
898             is = (i:i+nx-2);
899             patches.cs(:,:,:,:,i,j,k) = cs(is,js,ks,:);
900           end
901         end
902       end
903       patches.cs = reshape(patches.cs,nx-1,ny-1,nz-1,nc,[]);
```

Further, set a cunning left/right/bottom/top/front/back realisation of inter-patch coupling. The aim is to preserve symmetry in the system when also invoking `EdgyInt`. What this coupling does without `EdgyInt` is unknown. Use auto-replication.

```
913       mmx=(0:mx-1)'; mmy=0:my-1; mmz=shiftdim(0:mz-1,-1);
914       le = mod(mmx+mod(nx-2,mx),mx)+1;
915       patches.le = reshape(  le+mx*(mmy+my*mmz)  ,[],1);
916       ri = mod(mmx-mod(nx-2,mx),mx)+1;
917       patches.ri = reshape(  ri+mx*(mmy+my*mmz)  ,[],1);
918       bo = mod(mmy+mod(ny-2,my),my)+1;
919       patches.bo = reshape( 1+mmx+mx*(bo-1+my*mmz) ,[],1);
920       to = mod(mmy-mod(ny-2,my),my)+1;
921       patches.to = reshape( 1+mmx+mx*(to-1+my*mmz) ,[],1);
922       ba = mod(mmz+mod(nz-2,mz),mz)+1;
923       patches.ba = reshape( 1+mmx+mx*(mmy+my*(ba-1)) ,[],1);
924       fr = mod(mmz-mod(nz-2,mz),mz)+1;
925       patches.fr = reshape( 1+mmx+mx*(mmy+my*(fr-1)) ,[],1);
```

Issue warning if the ensemble is likely to be affected by lack of scale separation. [32]

```
933 if prod(ratio)*patches.nEnsem>0.9, warning( ...
934 'Probably poor scale separation in ensemble of coupled phase-shifts')
935 scaleSeparationParameter = ratio*patches.nEnsem
936 end
```

End the two if-statements.

```
942   end%if-else nEnsem>1
943 end%if not-empty(cs)
```

[32] **ToDo:** Need to justify this and the arbitrary threshold more carefully??

If parallel code then first assume this is not within an `spmd`-environment, and so we invoke `spmd...end` (which starts a parallel pool if not already started). At this point, the global `patches` is copied for each worker processor and so it becomes *composite* when we distribute any one of the fields. Hereafter, *all fields in the global variable* `patches` *must only be referenced within an* `spmd`*-environment.*[33]

```
if patches.parallel
  spmd
```

Second, decide which dimension is to be sliced among parallel workers (for the moment, do not consider slicing the ensemble). Choose the direction of most patches, biased towards the last.

```
  [~,pari]=max(nPatch+0.01*(1:3));
  patches.codist=codistributor1d(5+pari);
```

`patches.codist.Dimension` is the index that is split among workers. Then distribute the appropriate coordinate direction among the workers: the function must be invoked inside an `spmd`-group in order for this to work—so we do not need `parallel` in argument list.

```
  switch pari
    case 1, patches.x=codistributed(patches.x,patches.codist);
    case 2, patches.y=codistributed(patches.y,patches.codist);
    case 3, patches.z=codistributed(patches.z,patches.codist);
  otherwise
    error('should never have bad index for parallel distribution')
  end%switch
  end%spmd
```

If not parallel, then clean out `patches.codist` if it exists. May not need, but safer.

```
else% not parallel
  if isfield(patches,'codist'), rmfield(patches,'codist'); end
end%if-parallel
```

Fin

```
end% function
```

[33] If subsequently outside spmd, then one must use functions like `getfield(patches{1},'a')`.

References

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