Equation-free computational homogenisation with Dirichlet boundaries

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November 18, 2022

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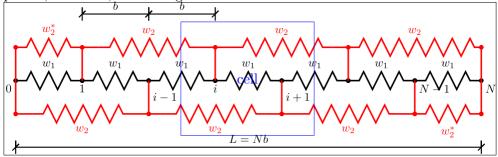
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Plot an example simulation in time generated by the patch scheme applied to macroscale toy elasticity through a medium with microscale heterogeneity.

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Figure 1: 1D arrangement of non-linear springs with connections to (a) next-to-neighbor node (Combescure 2022, Fig. 3(a)). The blue box is one cell of one period, width 2b, containing an odd and an even i.



Suppose the spatial microscale lattice is at rest at points x_i , with constant spacing b (Figure 1). With displacement variables $u_i(t)$, simulate the microscale lattice toy elasticity system with 2-periodicity: for p = 1, 2 (respectively black and red in Figure 1) and for every i,

$$\epsilon_i^p := \frac{1}{pb} (u_{i+p/2} - u_{i-p/2}), \quad \sigma_i^p := w_p'(\epsilon_i^p), \quad \frac{\partial^2 u_i}{\partial t^2} = \sum_{p=1}^2 \frac{1}{pb!} (\sigma_{i+p/2}^p - \sigma_{i-p/2}^p). \tag{1}$$

The system has a microscale heterogeneity via the different functions $w'_p(\epsilon) := \epsilon - M_p \epsilon^3 + \epsilon^5$ (Combescure 2022, §4):

- microscale instability with $M_1 := 2$ and $M_2 := 1$; and
- macroscale instability with $M_1 := -1$ and $M_2 := 3$.

1.1 Simulate heterogeneous toy elasticity systems

Set some physical parameters.

```
clear all
global b M vis i0 iN dFdt
b = 1 % separation of lattice points
N = 40 % # lattice steps in L
L = b*N
M = [0 0] % no cubic spring terms
M = [2 1] % small scale instability
M = [-1 3] % large scale instability
```

```
98 vis = 0
99 tol = 1e-9;
```

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dFdt = 0.02

Patch parameters: here nSubP is the number of cells, so lPatch is the distance from leftmost odd/even points to the rightmost odd/even points, respectively.

edgyInt = true

%nSubP = 4, nP = 3 108 H=L/nP 109 if edgyInt, ratio=2*b*(nSubP-2)/H, end

nSubP = 6, nP = 5 % gives ratio=1 for full-domain

%nP4ratio1=L/(2*b*(nSubP-2))

Establish the global data struct patches for the microscale heterogeneous lattice toy elasticity system (1). Solved on 2L-periodic domain, with 2*nP patches, and spectral interpolation to provide the edge-values of the inter-patch

coupling conditions.

124 global patches
125 configPatches1(@heteroToyE,[0 2*L],nan,2*nP ...
126 ,0,ratio,nSubP,'EdgyInt',edgyInt);

patches.x = patches.x-L+H/2;% shift so [0,L] is 2nd half of patches

%xGrid=squeeze(patches.x) % optionally disp the spatial grid
assert(abs(2*b-diff(patches.x(1:2)))<tol,'sub-patch grid config error
xx = patches.x+[-1 1]*b/2; % staggered sub-cell positions</pre>

Tasabian

1.2 Eigenvalues of the Jacobian
Set zero to be the reference equilibrium

Set zero to be the reference equilibrium in this linear problem. Put NaNs on the patch-edges.

if 0
u0 = [0*xx 0*xx];
u0([1 end],:,:,:)=nan;

i=find(~isnan(u0));
nJac=length(i)

Remove boundary conditions. i0=[]; iN=[];

Construct the Jacobian column-wise from the transform of a complete set of unit basis vectors (as this is linear problem at the moment).

```
dujdt=patchSys1(-1,uj);
       Jac(:,j)=dujdt(i);
161
     end
162
     Jac(abs(Jac)<tol)=0;</pre>
163
     figure(3),clf,spy(Jac)
164
     Find eigenvalues
     [evecs, evals] = eig(Jac);
170
     evals=diag(evals);
171
     [~,j]=sort( -real(evals)+0.0001*abs(imag(evals)) );
172
     evals=evals(j);
173
     evecs=evecs(:,j);
174
    leadingEvals=evals(1:18);
175
     Plot spectrum
        handle = plot(real(evals),imag(evals),'.');
181
        xlabel('real-part'), ylabel('imag-part')
182
        quasiLogAxes(handle,0.1,1);
183
        drawnow
184
     end%if compute eigenvalues
185
                  Set the initial conditions of a simulation. I choose to store odd i
    in u((i+1)/2,1,:) and even i in u(i/2,2,:), that is, array
                                    \mathbf{u} = egin{bmatrix} u_1 & u_2 \\ u_3 & u_4 \\ u_5 & u_6 \\ \vdots & \ddots \end{bmatrix}.
    u0 = 0*[\sin(pi/L*xx) -0.14*\cos(pi/L*xx)];
199
    u0 = u0+0.01*(rand(size(u0))-0.5);
200
    But, impose u_i = 0 at x = 0 which here I translate to mean that u_i = \dot{u}_i = 0
    for both x_i = \pm b/2. Slightly different to the left-end of Figure 1, but should
     be near enough. Here find both u, \dot{u} locations.
     i0=find(abs([xx xx])<0.6*b);
206
     u(i0)=0;
207
```

Jac=nan(nJac);

uj=u0; uj(i(j))=1;

for j=1:nJac

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Apply a set force at material originally at x=L, so start with $u_i=\dot{u}_i=0$ for both $x_i=L\pm b/2$. Subsequently apply an additional and increasing compression force on the points initially at x=L. Hmmm: but that is not quite isolating the two sides of x=L??

iN=find(abs([xx xx]-L)<0.6*b)
u(iN)=0;

Integrate some time using standard integrator.

```
tic
[ts,ust] = ode23(@patchSys1, 60*linspace(0,1,31), u0(:));
cpuIntegrateTime = toc
```

Plot space-time surface of the simulation We want to see the edge values of the patches, so interpolate and then adjoin a row of nans in between patches. Because of the odd/even storage we need to do a lot of permuting and reshaping.

vs = reshape(vs,[],length(ts));
Plot evolving function

```
figure(1),clf()
plot(xs(:),vs)
xlabel('space x')
ylabel('displacement u')
ylabel('velocity v')
legend(num2str(ts))
```

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

_

```
figure(2), clf()
266
      mesh(ts,xs(:),us)
267
      view(60,40), colormap(0.8*hsv)
268
      xlabel('time t'), ylabel('space x'), zlabel('u(x,t)')
269
      title(['patch ratio r = ' num2str(ratio)])
270
      drawnow
      figure(3), clf()
272
      mesh(ts,xs(:),vs)
273
      view(60,40), colormap(0.8*hsv)
      xlabel('time t'), ylabel('space x'), zlabel('v(x,t)')
      title(['patch ratio r = ' num2str(ratio)])
276
      drawnow
277
```

heteroToyE(): forced heterogeneous toy elasticity 1.3

This function codes the lattice heterogeneous toy elasticity inside the patches. Computes the time derivative at each point in the interior of a patch, output in ut.

```
function uvt = heteroToyE(t,uv,patches)
13
     global b M vis iO iN dFdt
```

14

Separate state vector into displacement and velocity fields.

```
u=uv(:,1:2,:,:); v=uv(:,3:4,:,:); % separate u and v=du/dt
```

Compute the two different strain fields, and also a first derivative for some optional viscosity.

```
eps2 = diff(u)/(2*b);
26
     eps1 = [u(:,2,:,:)-u(:,1,:,:) u([2:end 1],1,:,:)-u(:,2,:,:)]/b;
27
     eps1(end,2,:,:)=nan; % as this value is fake
28
          = [v(:,2,:,:)-v(:,1,:,:) \ v([2:end 1],1,:,:)-v(:,2,:,:)]/b;
29
     vx1(end,2,:,:)=nan; % as this value is fake
```

Set corresponding nonlinear stresses

```
sig2 = eps2-M(2)*eps2.^3+eps2.^5;
36
     sig1 = eps1-M(1)*eps1.^3+eps1.^5;
37
```

Preallocate output array, and fill in time derivatives of displacement and velocity, from velocity and gradient of stresses, respectively.

Maintain boundary value of u_i , \dot{u}_i by setting them both to be constant in time, for both $x_i = \pm b/2$. If i0 is empty, then no boundary condition is set.

```
56    uvt(i0)=0;
57    uvt(iN(3:4))=uvt(iN(3:4))-dFdt*t;
58    end% function
```

2 Eckhardt221004536: 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.

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

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

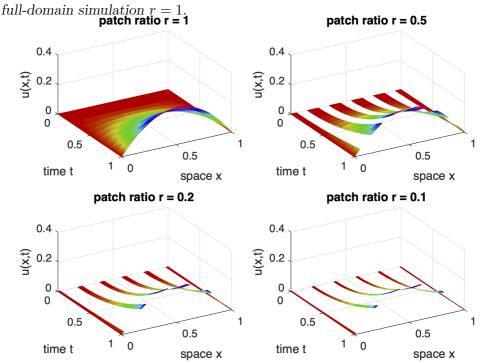
in terms of the centred difference operator δ . The system has a microscale heterogeneity via the coefficients $a_{i+1/2}$ which has some given known periodicity ϵ .

Here use period $\epsilon = 1/200$ (so that computation completes in seconds). The patch scheme computes only on a fraction r of the spatial domain, see Figure 2. 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 1/1200).

The smooth sine-forcing leads to errors that appear due to the integration tolerance of ode15s. The Eckhardt-forcing errors are then viewed as either due to boundary layers next to the Dirichlet boundaries, or equivalently due to

_

Figure 2: diffusion field u(x,t) of the patch scheme applied to the forced heterogeneous diffusive (2). Simulates for various patch ratios r including the



the lack of smoothness in the odd-periodic extensions of the forcing required to preserve the Dirichlet conditions.

2.1 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. 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.

```
82  mPeriod = 6
83  y = linspace(0,1,mPeriod+1)';
84  a = 1./(2-cos(2*pi*y(1:mPeriod)))
85  global microTimePeriod; microTimePeriod=0;
```

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

```
rEpsilon = 200
93
    dx = 1/(mPeriod*rEpsilon)
    nP = 5 \% the number of patches on [0 1]
    maxPeriodsPatch = rEpsilon/nP
    tol=1e-9;
97
    Loop to explore errors on various sized patches.
    nPPs = maxPeriodsPatch./[1 2 5 10 20 50 100];
103
104
```

nPPs = nPPs(nPPs>1)Us=[]; Uerr=0; % for storing results to compare

for iPP = 1:length(nPPs) nPeriodsPatch = nPPs(iPP)

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Establish the global data struct patches for the microscale heterogeneous lattice diffusion system (2) solved on 2-periodic domain, with 2*nP patches, and spectral interpolation to provide the edge-values of the inter-patch coupling conditions¹. 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).

```
ratio = nPeriodsPatch/maxPeriodsPatch
nSubP = nPeriodsPatch*mPeriod+2
global patches
configPatches1(@heteroDiffF,[0 2],nan,2*nP ...
    ,0,ratio,nSubP,'EdgyInt',true,'hetCoeffs',a);
patches.x = patches.x-1+1/(2*nP);% shift so [0,1] is 2nd half of patches.x
```

Set the forcing coefficients as the odd-periodic extensions, accounting for roundoff error in £2.

assert(abs(dx-diff(patches.x(1:2)))<tol, 'sub-patch-grid config error'

%x=squeeze(patches.x) % optionally disp the spatial grid

patches.f1=2*(patches.x-sign(patches.x).*patches.x.^2 ...

if 1 % odd-periodic extension of given forcing

⁺⁽patches.x>1).*(patches.x-1).^2*2); 142 patches.f2=2*0.5*sign(patches.x.*(1-patches.x)) ... 143

^{.*(}abs(patches.x.*(1-patches.x))>tol); 144 else% simple sine forcing give errors less than 2e-8 145 patches.f1=sin(pi*patches.x); 146

¹Curiously, for low-order interpolation—less than order 8—the error for large patches is larger than that for small patches

```
patches.f2=pi/2*sin(pi*patches.x);
147
    end%if
148
    %f1=squeeze(patches.f1)% optionally disp spatial pattern f1
149
    %f2=squeeze(patches.f2)% optionally disp spatial pattern f2
150
    Simulate Set the initial conditions of a simulation to be zero. Integrate to
    time 1 using standard integrators.
    u0 = 0*patches.x;
    [ts,us] = ode15s(@patchSys1, [0 1], u0(:));
161
    Plot space-time surface of the simulation We want to see the edge
    values of the patches, so adjoin a row of nans in between patches. For the field
    values (which are rows in us) we need to reshape, permute, interpolate to get
    edge values, pad with nans, and reshape again.
    xs = squeeze(patches.x);
174
    us = patchEdgeInt1( permute( reshape(us ...
175
         ,length(ts),nSubP,1,nPatch),[2 1 3 4]));
176
    us = squeeze(us);
177
    xs(end+1,:) = nan;
                          us(end+1,:,:) = nan;
178
    uss=reshape(permute(us,[1 3 2]),[],length(ts));
179
       Test the error in BC is negligible, for both when micro-grid point on
    boundary and when micro-grid points straddle boundary.
    i=[ max(find(xs<+tol)) min(find(xs>1-tol)) ];
188
    j=[ min(find(xs>-tol)) max(find(xs<1+tol)) ];</pre>
189
    maxBCerror=max(max( abs(uss(i,:)+uss(j,:))/2 ));
190
    assert(maxBCerror<tol,'BC failure')</pre>
191
       Plot a space-time surface of field values over the macroscale duration of
    the simulation.
    if iPP<=4 % only draw four subplots
199
      i=j(1):j(2);
200
      figure(1), if iPP==1, clf(), end
201
      subplot(2,2,iPP)
202
      mesh(ts,xs(i),uss(i,:))
203
```

xlabel('time t'), ylabel('space x'), zlabel('u(x,t)')

title(['patch ratio r = ' num2str(ratio)])

view(60,40), colormap(0.8*hsv)

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drawnow

end%if

At the end of the iPP-loop, store field from centre region of each patch for comparison.

```
i=nPeriodsPatch/2*mPeriod+1+(-mPeriod/2+1:mPeriod/2):
216
    Us(:,:,iPP)=squeeze(us(i,end,:));
217
    Xs=squeeze(patches.x(i,1,1,:));
218
    if iPP>1
       assert(norm(Xs-Xsp)<tol, 'sampling error in space')</pre>
220
       Uerr(iPP)=max(max(abs(squeeze(Us(:,:,iPP)-Us(:,:,1)))))
221
       end
222
    Xsp=Xs;
223
    end%for iPP
224
    ifOurCf2eps(mfilename) %optionally save figure
225
```

2.2 heteroDiffF(): forced heterogeneous diffusion

This function codes the lattice heterogeneous diffusion inside the patches. 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)
16
     global microTimePeriod
17
     dx = diff(patches.x(2:3));
                                   % space step
     i = 2:size(u,1)-1;
                           % interior points in a patch
                           % preallocate output array
     ut = nan+u;
     if microTimePeriod>0 % optional time fluctuations
        at = cos(2*pi*t/microTimePeriod)/30;
     else at=0; end
23
     ut(i,:,:,:) = diff((patches.cs(:,1,:)+at).*diff(u))/dx^2 ...
24
         +patches.f2(i,:,:,:)*t^2+patches.f1(i,:,:,:)*t;
25
   end% function
```

3 piEckhart1: example of 1D space-time heterogeneous diffusion via computational homogenisation with projective integration and small patches

Plot an example simulation in time generated by projective integration allied with the patch scheme applied to forced diffusion in a medium with microscale heterogeneity.

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

$$\frac{\partial u_i}{\partial t} = \frac{1}{dx^2} \delta[a_{i-1/2}(t)\delta u_i] + f_i(t), \tag{3}$$

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.

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

3.1 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.

```
82  mPeriod = 6
83  y = linspace(0,1,mPeriod+1)';
84  a = ( 3+cos(2*pi*y(1:mPeriod)) )/30
85  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.

```
patches.x = patches.x-1+1/(2*nP);% shift so [0,1] is 2nd half of patches.x
125
    assert(abs(dx-diff(patches.x(1:2)))<tol,'sub-patch-grid config error'
126
       Set the forcing coefficients as the odd-periodic extensions, accounting for
    roundoff error in f2.
    if 1 % odd-periodic extension of given forcing
134
    patches.f1=2*( patches.x-sign(patches.x).*patches.x.^2 ...
135
                   +(patches.x>1).*(patches.x-1).^2*2);
136
    patches.f2=2*0.5*sign(patches.x.*(1-patches.x)) ...
137
        .*(abs(patches.x.*(1-patches.x))>tol);
138
    else% simple sine forcing give errors less than ??
139
    patches.f1=sin(pi*patches.x);
140
    patches.f2=pi/2*sin(pi*patches.x);
141
    end%if
142
    %f1=squeeze(patches.f1)% optionally disp spatial pattern f1
143
    %f2=squeeze(patches.f2)% optionally disp spatial pattern f2
144
               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.
```

Establish the global data struct patches for the microscale heterogeneous lattice diffusion system (3) solved on 2-periodic macroscale domain, with 2*nP patches, and spectral interpolation to provide the edge-values of the inter-patch coupling conditions. Setting patches.EdgyInt true means the edge-values come from interpolating the opposite next-to-edge values of the patches (not

rEpsilon = 100

nPeriodsPatch = 2

the mid-patch values).

global patches

tol=1e-9:

dx = 1/(mPeriod*rEpsilon)

global microTimePeriod

microTimePeriod = 1/rEpsilon^2

ratio = nPeriodsPatch/(rEpsilon/nP)

configPatches1(@heteroDiffF,[0 2],nan,2*nP ...

,0,ratio,nSubP,'EdgyInt',true,'hetCoeffs',a);

nSubP = nPeriodsPatch*mPeriod+2

nP = 5 % the number of patches on [0 1]

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123

124

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

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tic

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 $\beta \approx \pi^2 A_0/h^2 \approx 400$ for patch width $h = r/N \approx 0.02$: use the formula from the Manual, with 50% extra, and rounded to the nearest multiple of the time micro-periodicity.

```
ts = linspace(0,1,11)
beta = pi^2*AO/(ratio/nP)^2 % slowest rate of fast modes
bT = 1.5*log(beta*diff(ts(1:2)))/beta
bT = max(10,round(bT/microTimePeriod))*microTimePeriod +1e-12
```

Time the projective integration simulation.

addpath('../../ProjInt')

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

Test the error in BC is negligible, for both when micro-grid point on boundary and when micro-grid points straddle boundary. For some reason the BC error climbs after t = 0.7—could it be ode45 quirk?

```
xs = squeeze(patches.x);
i=[ max(find(xs<+tol)) min(find(xs>1-tol)) ];
j=[ min(find(xs>-tol)) max(find(xs<1+tol)) ];</pre>
medianBCerror=median( abs(uss(:,i)+uss(:,j))/2 ,'omitnan')
maxBCerror=max(max( abs(uss(:,i)+uss(:,j))/2 ))
assert(maxBCerror<5e-5,'BC failure')</pre>
```

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

```
Xs=mean(xs);
Us=squeeze(mean( reshape(us,length(ts),[],2*nP), 2,'omitnan'));
I=nP:2*nP;
figure(1),clf
for k = 1:2, subplot(2,2,k)
```

```
mesh(ts,Xs(I),Us(:,I)')
  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.

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

heteroBurstF(): a burst of heterogeneous diffusion 3.2

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)

[ts,ucts] = ode45(@patchSys1,ti+(0:microTimePeriod:bT),ui(:) end

global microTimePeriod

References

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end

Combescure, Christelle (Nov. 2022). "Selecting Generalized Continuum Theories for Nonlinear Periodic Solids Based on the Instabilities of the Underlying Microstructure". In: Journal of Elasticity. ISSN: 1573-2681. DOI: 10.1007/s10659-022-09949-6 (cit. on p. 2).