Equation-free computational homogenisation with Dirichlet boundaries

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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].

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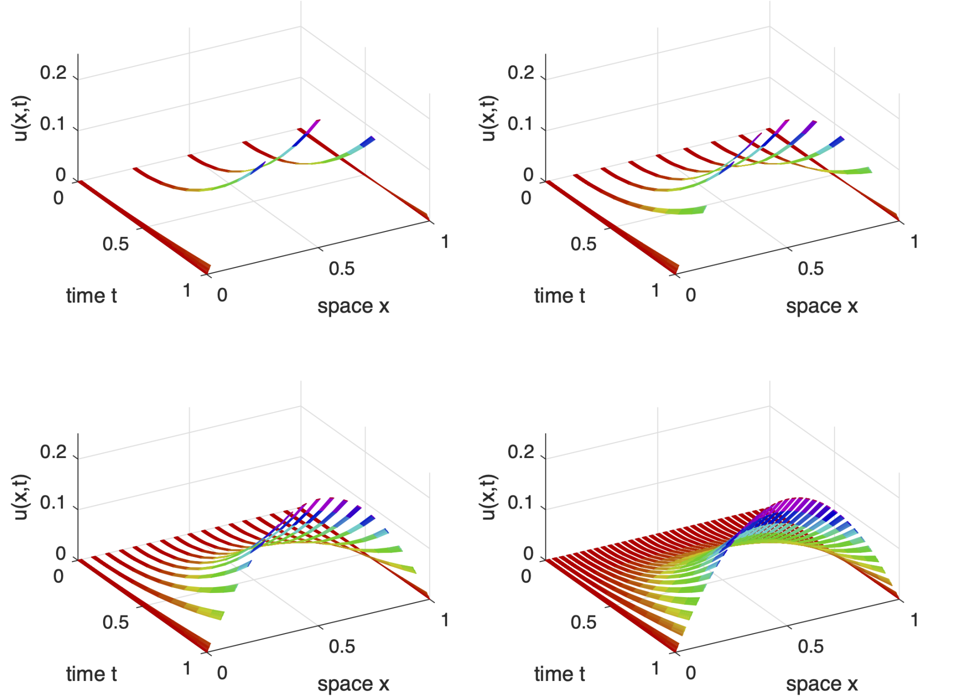
Figure 1: diffusion field $u(x,t)$ of the patch scheme applied to the forced heterogeneous diffusive (1). Simulate for $5, 9, 17, 33$ patches and compare to the full-domain simulation (65 patches, not shown).



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
sine-forcing error	0.0018	0.0009	0.0002	$1.6e{-5}$
parabolic-forcing error	$9.0e{-9}$	$3.7e{-9}$	$0.9e{-9}$	$0.06e{-9}$

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.

```
clear all
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],'equispaced',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 sinusoidal.

```
if 1 % 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. 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 `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);
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 figure
```

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')
```

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)
  global microTimePeriod
  % macroscale Dirichlet BCs
  u( 1 ,:,:, 1 )=0; % left-edge of leftmost is zero
  u(end,:,:,end)=0; % right-edge of rightmost is zero
  % interior forced diffusion
  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
  if microTimePeriod>0 % optional time fluctuations
     at = cos(2*pi*t/microTimePeriod)/30;
  else at=0; end
  ut(i,:,:,:) = diff((patches.cs(:,1,:)+at).*diff(u))/dx^2 ...
      +patches.f2(i,:,:,:)*t^2+patches.f1(i,:,:,:)*t;
end% function
```

2 EckhartEquilib: 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 Eckhardt2210.04536 §6.2.1.

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

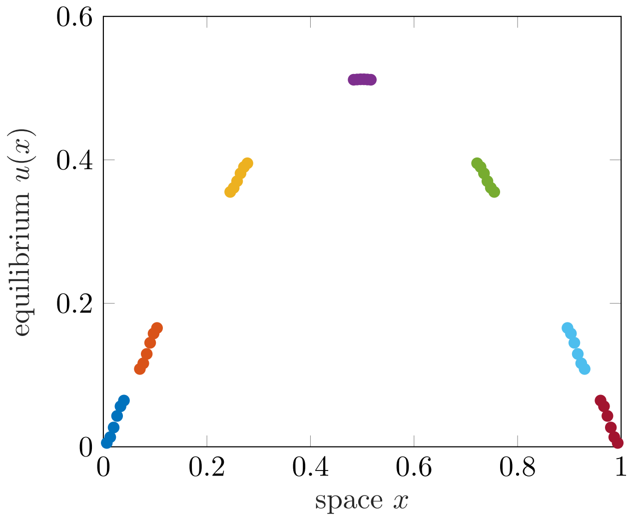


Figure 2: Equilibrium of the heterogeneous diffusion problem with forcing the same as that applied at time $t = 1$, and for relatively large $\epsilon = 0.04$ so we can see the patches. By default this code is for $\epsilon = 0.004$ where the microscale heterogeneity and patches are tiny.

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 = 250 % 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.

```
global patches
ordCC = 4
configPatches1(@heteroDiffF,[0 1],'chebyshev',nPatch ...
    ,ordCC,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
  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
```

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). Execute the function that invokes `fsolve`. For this linear problem, it is computationally quicker using a linear solver, but `fsolve` is quicker in human time, and generalises to nonlinear problems.

```
u = squeeze(execFsolve)
```

Then plot the equilibrium solution (Figure 2).

```
clf, plot(squeeze(patches.x),u,'.')
xlabel('space $x$'),ylabel('equilibrium $u(x)$')
```

Code to execute fsolve We code the function `execFsolve` to execute `fsolve` because easiest if a sub-function that computes the time derivatives has access to variables `u0` and `i`.

```
function [u,normRes] = execFsolve
global patches
```

Start the search from a zero field.

```
u0 = 0*patches.x;
```

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

```
u0([1 end],:,:,:) = nan;
i = find(~isnan(u0));
```

Seek the equilibrium, and report the norm of the residual.

```
[u0(i),res] = fsolve(@duidt,u0(i));
normRes = norm(res)
```

The aim is to zero the time derivatives `duidt` in the following function. First, insert the vector of variables into the patch-array of `u0`. Second, find the time derivatives via the patch scheme, and finally return a vector of those at the patch-internal points.

```
function res = duidt(ui)
  u = u0;   u(i) = ui;
  res = patchSys1(1,u);
  res = res(i);
end%function duidt
end%function execFsolve
```

Fin.

3 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 3 shows an example patch simulation.

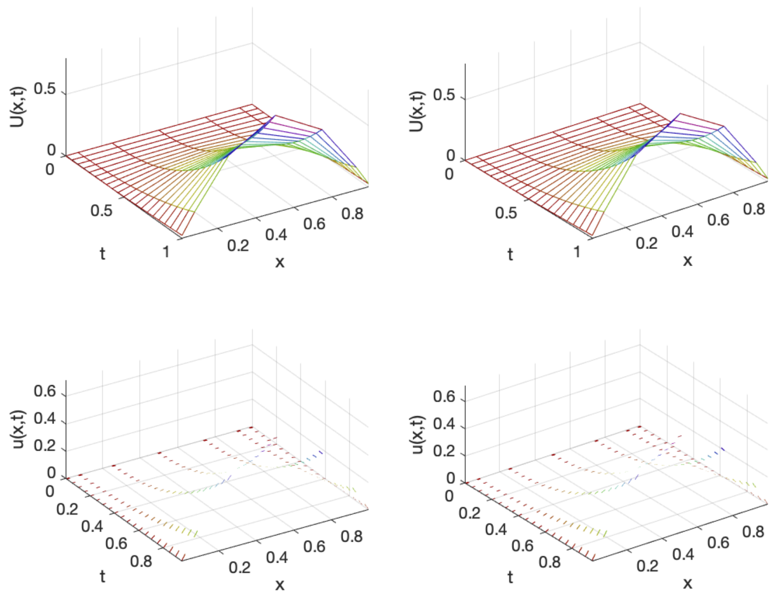
The approximate homogenised PDE is $U_t = A_0 U_{xx} + F$ with $U = 0$ at $x = 0, 1$. Its slowest mode is then $U = \sin(\pi x)e^{-A_0\pi^2 t}$. When $A_0 = 3.3524$ as in Eckhardt then the rate of evolution is about 33 which is relatively fast on the simulation time-scale of $T = 1$. Let's slow down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

Figure 3: 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.



only on a fraction 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.

```
clear all
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.

```
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
```

3.2 `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
```

References

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.

Eckhardt, Daniel and Barbara Verfürth (Oct. 2022). *Fully discrete Heterogeneous Multiscale Method for parabolic problems with multiple spatial and temporal scales*. Tech. rep. http://arxiv.org/abs/2210.04536 (cit. on pp. 1, 3, 9).