Equation-free computational homogenisation with Dirichlet boundaries

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1 `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

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

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 $\epsilon = 1/200$ (so that computation completes in seconds). The patch scheme computes only on a fraction r 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 1/1200).

patch ratio r	0.5	0.2	0.1	0.05
sine-forcing error	$0.5e{-8}$	$1.4e{-8}$	$1.8e{-8}$	$2.1e{-8}$
Eckhardt-forcing error	0.0018	0.0038	0.0046	0.0051

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

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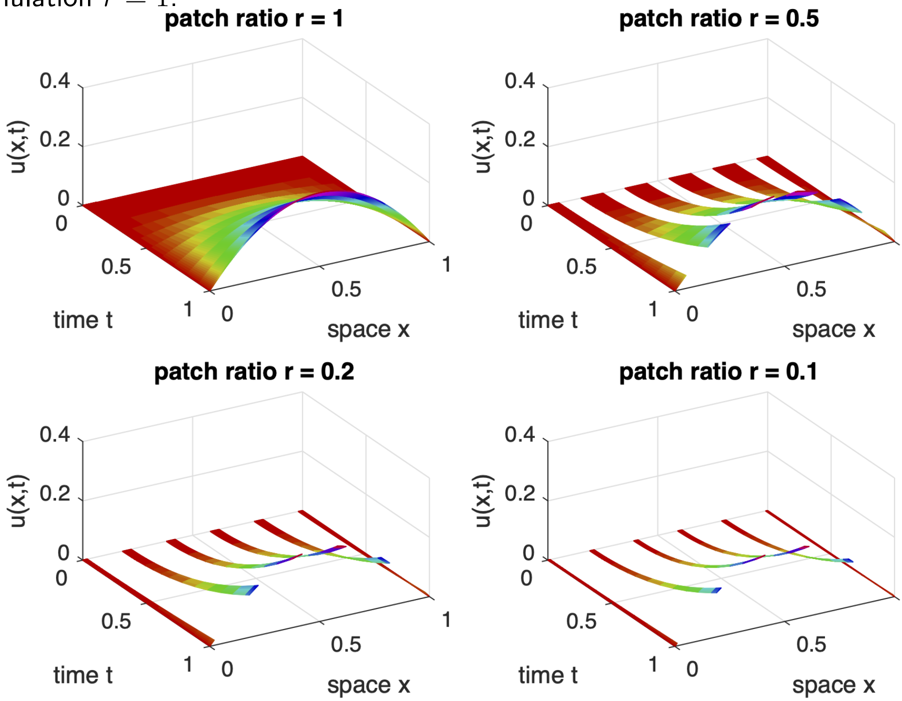
Figure 1: diffusion field $u(x,t)$ of the patch scheme applied to the forced heterogeneous diffusive (1). Simulates for various patch ratios r including the full-domain simulation $r = 1$.



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

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. 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.

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

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

```
rEpsilon = 200
dx = 1/(mPeriod*rEpsilon)
nP = 5 % the number of patches on [0 1]
maxPeriodsPatch = rEpsilon/nP
tol=1e-9;
```

Loop to explore errors on various sized patches.

```
nPPs = maxPeriodsPatch./[1 2 5 10 20 50 100];
nPPs = nPPs(nPPs>1)
Us=[]; Uerr=0;% for storing results to compare
for iPP = 1:length(nPPs)
nPeriodsPatch = nPPs(iPP)
```

Establish the global data struct `patches` for the microscale heterogeneous lattice diffusion system (1) solved on 2-periodic domain, with `2*nP` patches, and spectral interpolation to provide the edge-values of the inter-patch coupling conditions[1]. 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 patc
%x=squeeze(patches.x) % optionally disp the spatial grid
assert(abs(dx-diff(patches.x(1:2)))<tol,'sub-patch-grid config error'
```

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

```
if 1 % odd-periodic extension of given forcing
patches.f1=2*( patches.x-sign(patches.x).*patches.x.^2 ...
              +(patches.x>1).*(patches.x-1).^2*2 );
patches.f2=2*0.5*sign(patches.x.*(1-patches.x)) ...
    .*(abs(patches.x.*(1-patches.x))>tol);
else% simple sine forcing give errors less than 2e-8
patches.f1=sin(pi*patches.x);
```

[1] Curiously, 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);
end%if
%f1=squeeze(patches.f1)% optionally disp spatial pattern f1
%f2=squeeze(patches.f2)% optionally disp spatial pattern f2
```

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(:));
```

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,nPatch) ,[2 1 3 4]) );
us = squeeze(us);
xs(end+1,:) = nan;  us(end+1,:,:) = nan;
uss=reshape(permute(us,[1 3 2]),[],length(ts));
```

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)) ];
j=[ min(find(xs>-tol)) max(find(xs<1+tol)) ];
maxBCerror=max(max( abs(uss(i,:)+uss(j,:))/2 ));
assert(maxBCerror<tol,'BC failure')
```

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

```
if iPP<=4 % only draw four subplots
  i=j(1):j(2);
  figure(1), if iPP==1, clf(), end
  subplot(2,2,iPP)
  mesh(ts,xs(i),uss(i,:))
  view(60,40), colormap(0.8*hsv)
  xlabel('time t'), ylabel('space x'), zlabel('u(x,t)')
  title(['patch ratio r = ' num2str(ratio)])
  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);
Us(:,:,iPP)=squeeze(us(i,end,:));
Xs=squeeze(patches.x(i,1,1,:));
if iPP>1
   assert(norm(Xs-Xsp)<tol,'sampling error in space')
   Uerr(iPP)=max(max(abs(squeeze(Us(:,:,iPP)-Us(:,:,1)))))
   end
Xsp=Xs;
end%for iPP
ifOurCf2eps(mfilename) %optionally save figure
```

1.2 `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)
  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
  ut(i,:,:,:) = diff(patches.cs(:,1,:).*diff(u))/dx^2 ...
      +patches.f2(i,:,:,:)*t^2+patches.f1(i,:,:,:)*t;
end% function
```