First draft Moving Mesh documentation

AJR

September 4, 2021

Contents

1	mm1dBurgersExample: example of moving patches for Burgers'	
	PDE	1
	1.1 mmBurgersPDE(): Burgers PDE inside a moving mesh of patches	6
2	mmPatchSys1(): interface 1D space of moving patches to time	
	integrators	7
3	mm2dExample: example of moving patches in 2D for nonlinear	
	diffusion	13
	3.1 mmNonDiffPDE(): nonlinear diffusion PDE inside moving patches	18
4	mmPatchSys2(): interface 2D space of moving patches to time	
	integrators	19

1 mm1dBurgersExample: example of moving patches for Burgers' PDE

The code here shows one way to get started: a user's script may have the following three steps (left-right arrows denote function recursion).

- 1. configPatches1
- 2. ode15s integrator \leftrightarrow mmPatchSys1 \leftrightarrow user's PDE
- 3. process results

The simulation seems perfectly happy for the patches to move so that they overlap in the shock! and then separate again as the shock decays.

Establish global patch data struct to point to and interface with a function coding Burgers' PDE: to be solved on 1-periodic domain, with fifteen patches,

1

spectral interpolation couples the patches, each patch of half-size ratio 0.2, and with five microscale points forming each patch. Prefer EdgyInt as we suspect it performs better for moving meshes.

```
clear all
global patches
patches = configPatches1(@mmBurgersPDE,[0 1], nan, 15, 0, 0.2, 5 ...
,'EdgyInt',true);
patches.mmTime=0.8;
```

The above two amendments to patches should eventually be part of the configuration function.

Decide the moving mesh time parameter Here for $\epsilon = 0.02$.

patches.Xlim=[0 1];

36

- Would be best if the moving mesh was no stiffer than the stiffest microscale sub-patch mode. These would both be the zig-zag modes.
 - Here the mesh PDE is $X_t = (N^2/\tau) X_{jj}$ so its zig-zag mode decays with rate $4N^2/\tau$.
 - Here the patch width is h = 0.2/15 = 1/75, and so the microscale step is $\delta = h/4 = 1/300$. Hence the diffusion $u_t = \epsilon u_{xx}$ has zig-zag mode decaying at rate $4\epsilon/\delta^2$.

So, surely best to have $4N^2/\tau \lesssim 4\epsilon/\delta^2$, that is, $\tau \gtrsim N^2\delta^2/\epsilon \approx 0.1$.

- But also we do not want the slowest modes of the moving mesh to obfuscate the system's macroscale modes—the macroscale zig-zag.
 - The slowest moving mesh mode has wavenumber in j of $2\pi/N$, and hence rate of decay $(N^2/\tau)(2\pi/N)^2 = 4\pi^2/\tau$.
 - The fastest zig-zag mode of the system $U_t = \epsilon U_{xx}$ on step H has decay rate $4\epsilon/H^2$.

```
So best if 4\pi^2/\tau \gtrsim 4\epsilon/H^2, that is, \tau \lesssim \pi^2 H^2/\epsilon \approx 2. (Computations indicate need \tau < 0.8??)
```

Simulate in time Set usual sinusoidal initial condition. Add some microscale randomness that decays within time of 0.01, but also seeds slight macroscale variations.

```
83  u0 = 0.3+sin(2*pi*patches.x)+0.0*randn(size(patches.x));
84  N = size(patches.x,4)
85  D0 = zeros(N,1);
86  %ud=mmPatchSys1(0,[D0;u0(:)],patches);
87  %return
```

Simulate in time using a standard stiff integrator and the interface function mmPatchSys1() (Section 2).

```
tic
fts,us] = ode15s(@mmPatchSys1,linspace(0,0.8),[D0;u0(:)]);
function cpuTime = toc
```

Plots Choose whether to save some plots, or not.

```
global OurCf2eps
or OurCf2eps = false;
```

figure(1),clf

116

132

Plot the movement of the mesh, the centre of each patch, as a function of time: spatial domain horizontal, and time vertical.

```
Ds=us(:,1:N);

Xs=shiftdim(mean(patches.x),2);

plot(Xs+Ds,ts), ylabel('time t'),xlabel('space x')

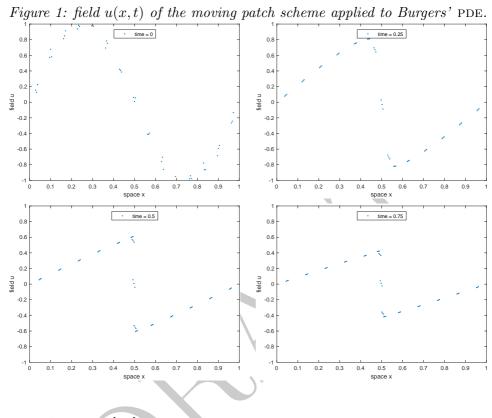
title('Burgers PDE: patch locations over time')

ifOurCf2eps([mfilename 'Mesh'])
```

Animate the simulation using only the microscale values interior to the patches: set x-edges to nan to leave the gaps. Figure 1 illustrates an example simulation in time generated by the patch scheme applied to Burgers' PDE.

```
us=us(:,N+1:end).';
us(abs(us)>2)=nan;
x0s=squeeze(patches.x); x0s([1 end],:)=nan;
%% section break to ease rerun of animation
figure(2),clf
```

uLim=[min(u0(:)) max(u0(:))]



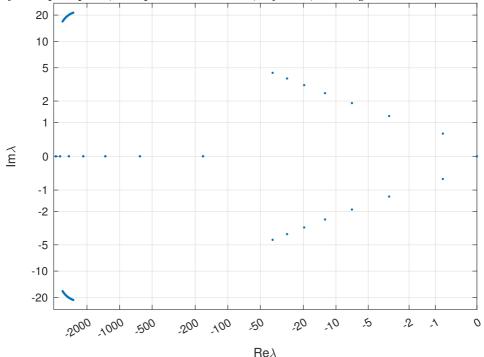
```
for i=1:length(ts)
138
      xs=x0s+Ds(i,:);
139
                 hpts=plot(xs(:),us(:,i),'.');
      if i == 1,
140
            ylabel('field u'), xlabel('space x')
            axis([0 1 uLim])
142
      else set(hpts,'XData',xs(:),'YData',us(:,i));
143
      end
144
      legend(['time = ' num2str(ts(i),2)],'Location','north')
145
      if rem(i,31)==1, ifOurCf2eps([mfilename num2str(i)]), end
146
      pause(0.09)
147
    end
148
    %%
149
```

Spectrum of the moving patch system Compute the spectrum based upon the linearisation about some state: u = constant with D = 0 are equilibria;

otherwise the computation is about a 'quasi-equilibrium' on the 'fast-time'. u0 = 0.1+0*sin(2*pi*patches.x);173 u0 = [zeros(N,1); u0(:)];174 f0 = mmPatchSys1(0,u0); 175 normf0=norm(f0) 176 But we must only use the dynamic variables, so let's find where they are. xs=patches.x; xs([1 end],:,:,:)=nan; 183 i=find(~isnan([zeros(N,1);xs(:)])); 184 nJac=length(i) 185 Construct Jacobian with numerical differentiation. deltau=1e-7; 191 Jac=nan(nJac); 192 for j=1:nJac 193 uj=u0; uj(i(j))=uj(i(j))+deltau; 194 fj = mmPatchSys1(0,uj); 195 Jac(:,j)=(fj(i)-f0(i))/deltau;196 end 197 Compute and plot the spectrum with non-linear axis scaling (Figure 2). eval=-sort(-eig(Jac)) 204 figure(3),clf 205 plot(asinh(real(eval)),asinh(imag(eval)),'.') 206 xlabel('Re\lambda'), ylabel('Im\lambda') 207 ticks=[1;2;5]*10.^(0:4); 208 ticks=sort([0;ticks(:);-ticks(:)]); 209 set(gca,'Xtick',asinh(ticks) ... 210 ,'XtickLabel',cellstr(num2str(ticks,4)) ... 211 ,'XTickLabelRotation',30) 212 set(gca,'Ytick',asinh(ticks) ... 213 ,'YtickLabel',cellstr(num2str(ticks,4))) 214 grid 215 ifOurCf2eps([mfilename 'Spec']) 216

Fin.

Figure 2: spectrum of the moving mesh Burgers' system (about u=0.1). The four clusters are: right, macroscale Burgers' PDE (complex conjugate pairs); left complex pairs, sub-patch PDE modes; left real, moving mesh modes.



1.1 mmBurgersPDE(): Burgers PDE inside a moving mesh of patches

For the evolving scalar field u(t,x), we code a microscale discretisation of Burgers' PDE $u_t = \epsilon u_{xx} - u u_x$, for say $\epsilon = 0.02$, when the patches of microscale lattice move with various velocities V.

```
function ut = mmBurgersPDE(t,u,M,patches)
epsilon = 0.02;
```

Generic input/output variables

- t (scalar) current time—not used here as the PDE has no explicit time dependence (autonomous).
- $u (n \times 1 \times 1 \times N)$ field values on the patches of microscale lattice.

- M a struct of the following components.
 - \forall $(1 \times 1 \times 1 \times N)$ moving velocity of the jth patch.
 - D $(1 \times 1 \times 1 \times N)$ displacement of the jth patch from the fixed spatial positions stored in patches.x—not used here as the PDE has no explicit space dependence (homogeneous).
- patches struct of patch configuration information.
- ut $(n \times 1 \times 1 \times N)$ output computed values of the time derivatives Du/Dt on the patches of microscale lattice.

Here there is only one field variable, and one in the ensemble, so for simpler coding of the PDE we squeeze them out (no need to reshape when via mmPatchSys1).

47

48

Burgers PDE In terms of the moving derivative $Du/Dt := u_t + Vu_x$ the PDE becomes $Du/Dt = \epsilon u_{xx} + (V - u)u_x$. So code for every patch that $\dot{u}_{ij} = \frac{\epsilon}{h^2}(u_{i+1,j} - 2u_{i,j} + u_{i-1,j}) + (V_j - u_{ij})\frac{1}{2h}(u_{i+1,j} - u_{i-1,j})$ at all interior lattice points.

```
dx=diff(patches.x(1:2)); % microscale spacing

i=2:size(u,1)-1; % interior points in patches

ut=nan+u; % preallocate output array

ut(i,:) = epsilon*diff(u,2)/dx^2 ...

+(V-u(i,:)).*(u(i+1,:)-u(i-1,:))/(2*dx);

end
```

2 mmPatchSys1(): interface 1D space of moving patches to time integrators

To simulate in time with moving 1D spatial patches we need to interface a user's time derivative function with time integration routines such as ode23 or PIRK2. This function mmPatchSys1() provides an interface. Patch edge values are determined by macroscale interpolation of the patch-centre or edge values. Microscale heterogeneous systems may be accurately simulated with this function via appropriate interpolation. Communicate patch-design variables

(??) either via the global struct patches or via an optional third argument (except that this last is required for parallel computing of spmd).

```
function dudt = mmPatchSys1(t,u,patches)
if nargin<3, global patches, end</pre>
```

Input

- u is a vector of length nPatch+nSubP·nVars·nEnsem·nPatch where there are nVars·nEnsem field values at each of the points in the nSubP×nPatch grid, and because of the moving mesh there are an additional nPatch patch displacement values at its start.
- t is the current time to be passed to the user's time derivative function.
- patches a struct set by configPatches1() with the following information used here.
 - .fun is the name of the user's function fun(t,u,M,patches) that computes the time derivatives on the patchy lattice, where the jth patch moves at velocity $M.V_j$ and at current time is displaced $M.D_j$ from the fixed reference position in .x. The array u has size $nSubP \times nVars \times nEnsem \times nPatch$. Time derivatives should be computed into the same sized array, then herein the patch edge values are overwritten by zeros.
 - .x is $nSubP \times 1 \times 1 \times nPatch$ array of the spatial locations x_i of the microscale grid points in every patch. Currently it *must* be an equi-spaced lattice on both macro- and microscales ??
 - Xlim is two element vector of the (periodic) spatial domain within which the patches are placed.

Output

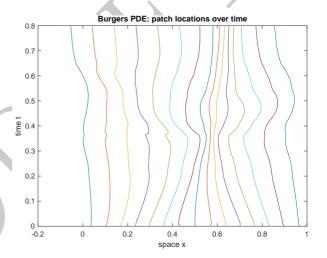
• dudt is a vector of of time derivatives, but with patch edge-values set to zero. It is of total length nPatch + nSubP · nVars · nEnsem · nPatch.

Alternative estimates of derivatives The moving mesh depends upon estimates of the second derivative of macroscale fields. Traditionally these are obtained from the macroscale variations in the fields. But with the patch scheme we can also estimate from the sub-patch fields. As yet we have little idea which is better. So here code three alternatives depending upon

Figure 3: patch locations as a function of time for the case subpatDerivstheselocations form a macroscale moving mesh.The shock here should be moving but appears to get pinned. These three are for $u_0 = 0.3 + \sin(2\pi x),$ spectral interpolation, $mesh \ \tau = 0.8$.

Burgers PDE: patch locations over time 0.8 0.7 0.6 0.4 0.3 0.2 0.1 -0.4 -0.2 0 0.2 0.4 0.6 0.8 space x

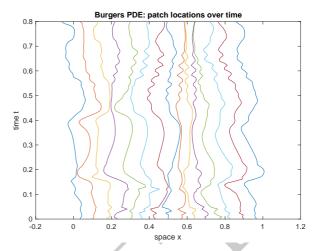
Figure 4: patch locations as a function of time for the case subpatDerivs = 2: these locations form a macroscale moving mesh. The shock here moves nicely, and the patches do not appear to overlap (much, or at all??). But what happens at time 0.4??



subpatDerivs = 2;

- subpatDerivs=0, implements classic moving mesh algorithm obtaining estimates of the 2nd derivative at each patch from the macroscale interpatch field—the moving shock is does not appear well represented (what about more patches?);
- subpatDerivs=2, obtains estimates of the 2nd derivative at each patch from the microscale sub-patch field (potentially subject to round-off problems)—but appears to track the shock OK;

Figure 5: patch locations as a function of time for the case subpatDerivs = 1: these locations form a macroscale moving mesh. The moving macroscale mesh of patches has some wacko oscillatory instability!



• subpatDerivs=1, estimates the first derivative from the microscale subpatch field (I expect round-off negligible), and then using macroscale differences to estimate the 2nd derivative at points mid-way between patches—seems to be subject to weird mesh oscillations.

Preliminaries Extract the nPatch displacement values from the start of the vectors of evolving variables. Reshape the rest as the fields u in a 4D-array, and sets the edge values from macroscale interpolation of centre-patch values. ?? describes patchEdgeInt1().

Moving mesh velocity Developing from standard moving meshes for PDEs (Budd et al. 2009, Huang & Russell 2010, e.g.), we follow Maclean, Bunder, Kevrekidis & Roberts (2021). There exists a set of macro-scale mesh points $X_j(t) := X_j^0 + D_j(t)$ (at the centre) of each patch with associated field values, say $U_j(t) := \overline{u_{ij}(t)}$.

```
181 X = mean(patches.x,1)+M.D;
182 if subpatDerivs==0, U = mean(u,1); end
```

Then for every patch j we set $H_j := X_{j+1} - X_j$ for periodic patch indices j

```
189  j=1:N; jp=[2:N 1]; jm=[N 1:N-1];
190  H = X(:,:,:,jp)-X(:,:,:,j);
```

H(N) = H(N) + diff(patches.Xlim);

we discretise a moving mesh PDE for node locations X_j with field values U_j via the second derivative estimate

$$U_j'' := \frac{2}{H_j + H_{j-1}} \left[\frac{U_{j+1} - U_j}{H_j} - \frac{U_j - U_{j-1}}{H_{j-1}} \right]. \tag{1a}$$

Here $\mathtt{U2} := \overset{\longleftarrow}{U}_{j}^{\prime\prime},$

191

204

205

206

207

208

228

229

230

231

232

233

234

switch subpatDerivs

Alternatively, use the sub-patch field to determine the second derivatives. It should be more accurate, unless round-off error becomes significant. However, it may focus too much on the microscale, and not enough on the macroscale variation.

- In the case of non-edgy interpolation, since we here use near edge-values, the derivative is essentially a numerical derivative of the interpolation scheme.
- In the case of edgy-interpolation, and if periodic heterogeneous microstructure, then we must have an even number of periods in every patch so that the second differences steps are done over a whole number of micro-scale periods.

```
case 2
  idel=floor((nx-1)/2);
  dx=diff(patches.x([1 idel+1]));
  U2=diff(u(1:idel:nx,:,:,:),2,1)/dx^2;
  if rem(nx,2)==0 % use average when even sub-patch points
     U2=( U2+diff(u(2:idel:nx,:,:,:),2,1)/dx^2 )/2;
  end%if nx even
```

Alternatively, use the sub-patch field to determine the first derivatives at each patch, and then a macroscale derivative to determine second derivative at

259

260

278

279

280

281

292

mid-gaps inter-patch. The sub-patch first derivative is a numerical estimate of the derivative of the inter-patch interpolation scheme as it only uses edge-values, values which come directly from the patch interpolation scheme.

Compute a norm over ensemble and all variables (arbitrarily?? chose the mean square norm here, so here U2 denotes both 2nd derivative and the square, here U2 := $\|\vec{U}_{j}^{"}\|^{2}$).

Having squeezed out all microscale information, the coefficient

$$\alpha := \max \left\{ 1, \left[\frac{1}{b-a} \sum_{j} H_{j-1} \frac{1}{2} \left(U_{j}^{"2/3} + U_{j-1}^{"2/3} \right) \right]^{3} \right\}$$
 (1b)

Rather than $\max(1,\cdot)$ surely better to use something smooth like $\sqrt{1+\cdot^2}$??

```
if subpatDerivs==1 % mid-point integration
  alpha = sum( H.*U2.^(1/3) )/sum(H);
  else % trapezoidal integration
  alpha = sum( H(jm).*( U2(j).^(1/3)+U2(jm).^(1/3) ))/2/sum(H);
  end%if
%alpha = max(1,alpha^3);
  alpha = sqrt(1+alpha^6);
```

Then the importance function (alternatively at patches or at mid-gap interpatch)

$$\rho_j := \left(1 + \frac{1}{\alpha} U_j''^2\right)^{1/3},\tag{1c}$$

rho = $(1+U2/alpha).^(1/3)$;

For every patch, we move all micro-grid points according to the following velocity of the notional macro-scale node of that patch:

$$V_j := \frac{dX_j}{dt} = \frac{(N-1)^2}{2\rho_j \tau} \left[(\rho_{j+1} + \rho_j) H_j - (\rho_j + \rho_{j-1}) H_{j-1} \right]. \tag{1d}$$

Control overlapping of patches? Surely cannot yet be done because the interpolation is in index space, so that adjoining patches generally have different field values interpolated to their edges. Need to interpolate in physical space in order to get the interpolated field to 'merge' adjoining patches.

Evaluate system differential equation Ask the user function for the advected time derivatives on the moving patches, overwrite its edge values with the dummy value of zero (since ode15s chokes on NaNs), then return to the user/integrator as a vector.

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

Fin.

336

337

338

3 mm2dExample: example of moving patches in 2D for nonlinear diffusion

The code here shows one way to use moving patches in 2D. However, mmPatchSys2() has far too many ad hoc assumptions, so fix those before exploring predictions here.

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, each patch of half-size ratio 0.4?? (relatively large for visualisation), and with 5×5 points forming each patch. Roberts et al. (2014) established that this scheme is consistent with the PDE (as the patch spacing decreases). Prefer EdgyInt as we suspect it performs better for moving meshes.

```
clear all
29
   global patches
30
   nxy=5
31
   Nx=9, Ny=7
32
   patches = configPatches2(@mmNonDiffPDE,[-3 3 -2 2], nan ...
33
        , [Nx Ny], 0, 0.2, nxy ,'EdgyInt',true);
   patches.mmTime=1;
   patches.Xlim=[-3 3 -2 2];
36
   Npts = Nx*Ny;
37
```

The above two amendments to patches should eventually be part of the configuration function.

Decide the moving mesh time parameter

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

```
84  u0 = exp(-patches.x.^2-patches.y.^2);
85  u0 = u0.*(0.9+0.0*rand(size(u0))) +0.001;
86  D0 = zeros(2*Npts,1);
```

Integrate in time to t=2 using standard functions. In Matlab ode15s would be natural as the patch scheme is naturally stiff, but ode23 is quicker (Maclean, Bunder & Roberts 2021, Fig. 4). Ask for output at non-uniform times because the diffusion slows.

```
disp('Simulating nonlinear diffusion h_t=(h^3)_xx+(h^3)_yy')
tic
fig. [ts,us] = ode23(@mmPatchSys2,2*linspace(0,1).^2,[D0;u0(:)]);
cpuTime = toc
```

Plots Choose whether to save some plots, or not.

```
global OurCf2eps
ourCf2eps = true;
```

Extract data from time simulation. Be wary that the patch-edge values do not change from initial, so either set to NaN, or set via interpolation.

```
nTime=length(ts);
115
    Ds=reshape(us(:,1:2*Npts).',1,1,Nx,Ny,2,nTime);
116
    us=reshape(us(:,2*Npts+1:end).',nxy,nxy,Nx,Ny,nTime);
117
    us([1 end],:,:)=nan; us(:,[1 end],:,:)=nan; % nan edges
118
       Choose macro-mesh plot or micro-surf-patch plots.
    if 1
125
    Plot the movement of the mesh, with the field vertical, at the centre of each
    patch.
    %% section marker for macro-mesh plot execution
132
    figure(1),clf, colormap(0.8*hsv)
133
    Us=shiftdim( mean(mean(us,1,'omitnan'),2,'omitnan')
134
    Xs=shiftdim(mean(patches.x),4);
135
    Ys=shiftdim(mean(patches.y),4);
136
    for k=1:nTime
137
      Xk=Xs+shiftdim(Ds(:,:,:,:,1,k),2);
138
      Yk=Ys+shiftdim(Ds(:,:,:,:,2,k),2);
139
      if k==1.
140
        hand=mesh(Xk,Yk,Us(:,:,k));
141
        ylabel('space y'),xlabel('space x'),zlabel('mean field U')
        axis([patches.Xlim 0 1]), caxis([0 1])
143
        colorbar
144
        if 0, view(0,90) % vertical view
145
        else view(-25,60) % 3D perspective
146
        end
147
      else
148
        set(hand, 'XData', Xk, 'YData', Yk ...
149
            ,'ZData',Us(:,:,k),'CData',Us(:,:,k))
150
      end
151
      legend(['time =' num2str(ts(k),4)],'Location','north')
152
      if rem(k,31)==1, ifOurCf2eps([mfilename num2str(k)]), end
153
      pause(0.05)
154
    end% for each time
155
    else%if macro-mesh or micro-surf
156
    Plot the movement of the patches, with the field vertical in each patch.
    % section marker for patch-surf plot execution
163
```

figure(2),clf, colormap(0.8*hsv)

164

```
xs=reshape(patches.x,nxy,1,Nx,1);
165
    ys=reshape(patches.y,1,nxy,1,Ny);
166
    for k=1:nTime
167
      xk=xs+0*ys+Ds(:,:,:,:,1,k);
168
      yk=ys+0*xs+Ds(:,:,:,:,2,k);
169
      uk=reshape(permute(us(:,:,:,k),[1 3 2 4]),nxy*Nx,nxy*Ny);
170
      xk=reshape(permute(xk,[1 3 2 4]),nxy*Nx,nxy*Ny);
      yk=reshape(permute(yk,[1 3 2 4]),nxy*Nx,nxy*Ny);
172
      if k==1,
173
        hand=surf(xk,yk,uk);
174
        ylabel('space y'),xlabel('space x'),zlabel('field u(x,y,t)')
175
        axis([patches.Xlim 0 1]), caxis([0 1])
176
        colorbar
      else
178
        set(hand,'XData',xk,'YData',yk,'ZData',uk,'CData',uk)
179
      end
180
      legend(['time =' num2str(ts(k),4)],'Location','north')
181
       if rem(k,31)==1, ifOurCf2eps([mfilename num2str(k)]), end
182
      pause(0.05)
183
    end% for each time
184
    %%
185
    end%if macro-mesh or micro-surf
```

Spectrum of the moving patch system Compute the spectrum based upon the linearisation about some state: u = constant with D = 0 are equilibria; otherwise the computation is about a 'quasi-equilibrium' on the 'fast-time'.

```
u00 = 0.1
213
    u0 = u00+0.1*exp(-patches.x.^2-patches.y.^2);
214
    u0([1 end],:,:,:)=nan; u0(:,[1 end],:,:)=nan;
215
    u0 = [zeros(2*Npts,1); u0(:)];
216
    f0 = mmPatchSys2(0,u0);
217
    normf0=norm(f0)
218
```

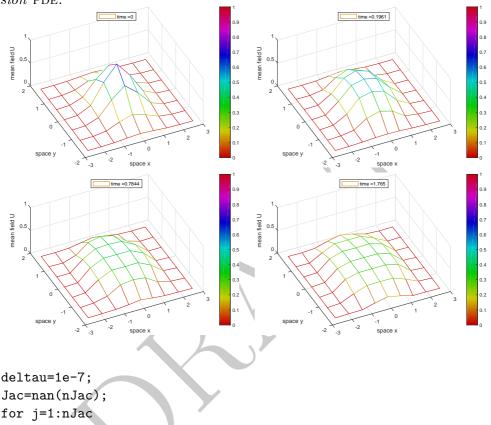
But we must only use the dynamic variables, so let's find where they are.

```
i=find(~isnan( u0(:) ));
225
    nJac=length(i)
226
```

186

Construct Jacobian with numerical differentiation.

Figure 6: field u(x,t) of the moving patch scheme applied to nonlinear diffusion PDE.



Compute and plot the spectrum with non-linear axis scaling (Figure 7).

```
245  eval=eig(Jac);
246  k=find(abs(imag(eval))<1e-6);
247  eval(k)=real(eval(k));
248  [~,k]=sort(-real(eval));
249  eval=eval(k);
250  nZero = sum(abs(real(eval))<1e-6)
251  nSlow = sum(-3*u00^2*300<real(eval))-nZero</pre>
```

```
eSlow = eval(nZero+(1:2:nSlow))
252
    eFast = eval([nZero+nSlow+1 end])
253
    figure(3),clf
254
    plot(asinh(real(eval)),asinh(imag(eval)),'.')
255
    xlabel('Re\lambda'), ylabel('Im\lambda')
256
    ticks=[1;2;5]*10.^(0:6);
257
    ticks=sort([0;ticks(:);-ticks(:)]);
258
    set(gca,'Xtick',asinh(ticks) ...
259
        ,'XtickLabel',cellstr(num2str(ticks,4))
260
        ,'XTickLabelRotation',30)
261
    set(gca,'Ytick',asinh(ticks) ...
262
        ,'YtickLabel',cellstr(num2str(ticks,4)))
263
    grid
264
    ifOurCf2eps([mfilename 'Spec'])
265
       Fin.
```

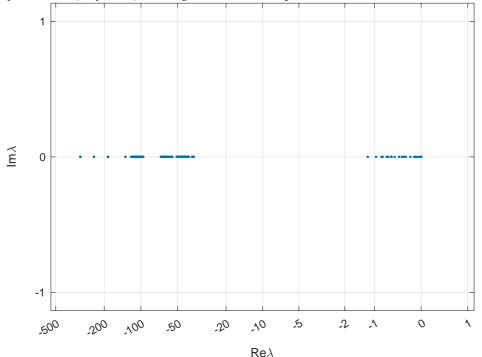
3.1 mmNonDiffPDE(): nonlinear diffusion PDE inside moving patches

As a microscale discretisation of $u_t = \overset{\checkmark}{V} \vec{\nabla} u + \nabla^2(u^3)$, code $\dot{u}_{ijkl} = \cdots +$

```
\frac{1}{\delta x^2} (u_{i+1,i,k,l}^3 - 2u_{i,i,k,l}^3 + u_{i-1,i,k,l}^3) + \frac{1}{\delta v^2} (u_{i,i+1,k,l}^3 - 2u_{i,i,k,l}^3 + u_{i,i-1,k,l}^3).
   function ut = mmNonDiffPDE(t,u,M,patches)
13
      if nargin<3, global patches, end
14
      u = squeeze(u); % reduce to 4D
      Vx = shiftdim(M.Vx,2); % omit two singleton dimens
      Vy = shiftdim(M.Vy,2); % omit two singleton dimens
      dx = diff(patches.x(1:2));  % microgrid spacing
      dy = diff(patches.y(1:2));
      i = 2:size(u,1)-1; j = 2:size(u,2)-1; % interior patch points
      ut = nan+u;  % preallocate output array
      ut(i,j,:,:) = ...
          +Vx.*(u(i+1,j,:,:)-u(i-1,j,:,:))/(2*dx) ...
23
          +Vy.*(u(i,j+1,:,:)-u(i,j-1,:,:))/(2*dy) ...
          +diff(u(:,j,:,:).^3,2,1)/dx^2...
25
          +diff(u(i,:,:,:).^3,2,2)/dy^2;
26
```

end

Figure 7: spectrum of the moving mesh 2D diffusion system (about u = 0.1). The clusters are: right real, macroscale diffusion modes with some neutral mesh deformations; left real, moving mesh and sub-patch modes.



4 mmPatchSys2(): interface 2D space of moving patches to time integrators

Beware ad hoc assumptions In an effort to get started, I have just made some plausible generalisations from the 1D code to this 2D code. Probably lots of details are poor??

To simulate in time with 2D patches moving in space we need to interface a users time derivative function with time integration routines such as ode23 or PIRK2. This function mmPatchSys2() provides an interface. Patch edge values are determined by macroscale interpolation of the patch-centre or edge values. Microscale heterogeneous systems may be accurately simulated with this function via appropriate interpolation. Communicate patch-design variables (??) either via the global struct patches or via an optional third argument (except that this last is required for parallel computing of spmd).

```
function dudt = mmPatchSys2(t,u,patches)
if nargin<3, global patches, end</pre>
```

Input

30

31

- u is a vector of length $2 \cdot \operatorname{prod}(\operatorname{nPatch}) + \operatorname{prod}(\operatorname{nSubP}) \cdot \operatorname{nVars} \cdot \operatorname{nEnsem} \cdot \operatorname{prod}(\operatorname{nPatch})$ where there are $\operatorname{nVars} \cdot \operatorname{nEnsem}$ field values at each of the points in the $\operatorname{nSubP}(1) \times \operatorname{nSubP}(2) \times \operatorname{nPatch}(1) \times \operatorname{nPatch}(2)$ grid.
- t is the current time to be passed to the user's time derivative function.
- patches a struct set by configPatches2() with the following information used here.
 - .fun is the name of the user's function fun(t,u,M,patches) that computes the time derivatives on the patchy lattice, where the (I,J)th patch moves at velocity $(M.Vx_I,M.Vy_J)$ and at current time is displaced $(M.Dx_I,M.Dy_J)$ from the fixed reference positions in .x and .y. The array u has size nSubP(1) × nSubP(2) × nVars × nEsem × nPatch(1) × nPatch(2). Time derivatives must be computed into the same sized array, although herein the patch edge-values are overwritten by zeros.
 - .x is $nSubP(1) \times 1 \times 1 \times 1nPatch(1) \times 1$ array of the spatial locations x_i of the microscale (i, j)-grid points in every patch. Currently it must be an equi-spaced lattice on both macro- and micro-scales??
 - .y is similarly $1 \times nSubP(2) \times 1 \times 1 \times 1 \times nPatch(2)$ array of the spatial locations y_j of the microscale (i, j)-grid points in every patch. Currently it must be an equi-spaced lattice on both macro- and micro-scales.
 - .Xlim ??

Output

• dudt is a vector/array of of time derivatives, but with patch edge-values set to zero. It is of total length $2 \cdot prod(nPatch) + prod(nSubP) \cdot nVars \cdot nEnsem \cdot prod(nPatch)$ and the same dimensions as u.

Extract the $2 \cdot prod(nPatch)$ displacement values from the start of the vectors of evolving variables. Reshape the rest as the fields u in a 6D-array, and sets the edge values from macroscale interpolation of centre-patch values. ?? describes patchEdgeInt2().

```
104  Nx = size(patches.x,5);
105  Ny = size(patches.y,6);
106  nM = Nx*Ny;
107  M.Dx = reshape(u( 1:nM ),[1 1 1 1 Nx Ny]);
108  M.Dy = reshape(u(nM+1:2*nM),[1 1 1 1 Nx Ny]);
109  u = patchEdgeInt2(u(2*nM+1:end),patches);
```

Moving mesh velocity Developing from standard moving meshes for PDEs (Budd et al. 2009, Huang & Russell 2010, e.g.), we follow Maclean, Bunder, Kevrekidis & Roberts (2021), and generalise ad hoc to 2D?? There exists a set of macro-scale mesh points $(X_{IJ}(t), Y_{IJ}(t)) := (X_{IJ}^0 + Dx_{IJ}(t), Y_{IJ}^0 + Dy_{IJ}(t))$ (at the centre) of each patch with associated field values, say $U_{IJ}(t) := \overline{u_{ijIJ}(t)}$. And remove the two microscale dimensions from the front of the arrays, so they are 4D arrays.

```
128 X = shiftdim( mean(patches.x,1)+M.Dx ,2);
129 Y = shiftdim( mean(patches.y,2)+M.Dy ,2);
130 U = shiftdim( mean(mean(u,1,'omitnan'),2,'omitnan') ,2);
131 %Uz=squeeze(U)
```

Then for every patch (I, J) we set $H_{IJ}^{pq} :=$ the qth spatial component of the step to the next patch in the pth index direction, for periodic patch indices (I, J),

```
I=1:Nx; Ip=[2:Nx 1]; Im=[Nx 1:Nx-1];
140
    J=1:Ny; Jp=[2:Ny 1]; Jm=[Ny 1:Ny-1];
141
    Hix = X(:,:,Ip,J)-X(:,:,I,J);
142
    Hiy = Y(:,:,Ip,J)-Y(:,:,I,J);
143
    Hjx = X(:,:,I,Jp)-X(:,:,I,J);
144
    H_{jy} = Y(:,:,I,J_p)-Y(:,:,I,J);
145
    Hix(:,:,Nx,:) = Hix(:,:,Nx,:) + diff(patches.Xlim(1:2));
146
    Hjy(:,:,:,Ny) = Hjy(:,:,:,Ny) + diff(patches.Xlim(3:4));
147
```

we discretise a moving mesh PDE for node locations (X_{IJ}, Y_{IJ}) with field values U_{IJ} via the second derivatives estimates ??

$$U_j'' := \frac{2}{H_j + H_{j-1}} \left[\frac{U_{j+1} - U_j}{H_j} - \frac{U_j - U_{j-1}}{H_{j-1}} \right]. \tag{2a}$$

First, compute first derivatives at $(I + \frac{1}{2}, J)$ and $(I, J + \frac{1}{2})$ respectively.

```
Ux = (U(:,:,Ip,J)-U(:,:,I,J))./Hix(:,:,I,J); %ux=squeeze(Ux)
Uy = (U(:,:,I,Jp)-U(:,:,I,J))./Hjy(:,:,I,J); %uy=squeeze(Uy)
```

Second, compute second derivative matrix, without assuming symmetry because the derivatives in space are not quite the same as the derivatives in indices. The mixed derivatives are at $(I + \frac{1}{2}, J + \frac{1}{2})$, so average to get at patch locations.

```
Uxx = (Ux(:,:,I,J)-Ux(:,:,Im,J))*2./(Hix(:,:,I,J)+Hix(:,:,Im,J));
Uyy = (Uy(:,:,I,J)-Uy(:,:,I,Jm))*2./(Hjy(:,:,I,J)+Hjy(:,:,I,Jm));
Uyx = (Uy(:,:,Ip,J)-Uy(:,:,I,J))./Hix(:,:,I,J);
```

Uxy = (Ux(:,:,I,Jp)-Ux(:,:,I,J))./Hjy(:,:,I,J);Uyx = (Uyx(:,:,I,J)+Uyx(:,:,Im,J)+Uyx(:,:,I,Jm)+Uyx(:,:,Im,Jm))/4;

191

192

193

194

195

212

213

215

216

217

Uxy = (Uxy(:,:,I,J)+Uxy(:,:,Im,J)+Uxy(:,:,I,Jm)+Uxy(:,:,Im,Jm))/4;

179 %uxx=squeeze(Uxx),uyy=squeeze(Uyy),uxy=squeeze(Uxy),uyx=squeeze(Uyx),

And compute its norm over all variables and ensembles (arbitrarily?? chose the mean square norm here, using abs.^2 as they may be complex), shifting the variable and ensemble dimensions out of the result to give 2D array of values, one for each patch (use shiftdim rather than squeeze as users may invoke a 1D array of 2D patches, as in channel dispersion).

Having squeezed out all microscale information, the global moderating coefficient in 1D??

$$\alpha := \max \left\{ 1, \left[\frac{1}{b-a} \sum_{j} H_{j-1} \frac{1}{2} \left(U_{j}^{"2/3} + U_{j-1}^{"2/3} \right) \right]^{3} \right\}$$
 (2b)

generalises to an integral over approximate parallelograms in 2D?? (area approximately?? determined by cross-product). Rather than $\max(1,\cdot)$ surely better to use something smooth like $\sqrt{(1+\cdot^2)}$??

Then the importance function at each patch is the 2D array

$$\rho_j := \left(1 + \frac{1}{\alpha} U_j''^2\right)^{1/3},$$
(2c)

rho = $(1+U2/alpha).^(1/3);$

227

246

247

248

249

250

251

252

253

Fin.

For every patch, we move all micro-grid points according to the following velocity of the notional macro-scale node of that patch: (Since we differentiate the importance function, maybe best to compute it above at half-grid points of the patches—aka a staggered scheme??)

$$V_j := \frac{dX_j}{dt} = \frac{(N-1)^2}{2\rho_j \tau} \left[(\rho_{j+1} + \rho_j) H_j - (\rho_j + \rho_{j-1}) H_{j-1} \right]. \tag{2d}$$

Is the Nx and Ny correct here?? And are the derivatives appropriate since these here are scaled index derivatives, not actually spatial derivatives??

Evaluate system differential equation Ask the user function for the time derivatives computed in the array, overwrite its edge values with the dummy value of zero (as ode15s chokes on NaNs), then return to the user/integrator as same sized array as input.

```
268  dudt = patches.fun(t,u,M,patches);
269  dudt([1 end],:,:,:,:) = 0;
270  dudt(:,[1 end],:,:,:,:) = 0;
271  dudt=[M.Vx(:); M.Vy(:); dudt(:)];
```

References 24

References

Budd, C. J., Huang, W. & Russell, R. D. (2009), 'Adaptivity with moving grids', *Acta Numerica* **18**, 111–241.

- Huang, W. & Russell, R. D. (2010), Adaptive moving mesh methods, Vol. 174, Springer Science & Business Media.
- Maclean, J., Bunder, J. E., Kevrekidis, I. G. & Roberts, A. J. (2021), Adaptively detect and accurately resolve macro-scale shocks in an efficient equation-free multiscale simulation, Technical report, University of Adelaide.
- Maclean, J., Bunder, J. E. & Roberts, A. J. (2021), 'A toolbox of equation-free functions in matlab/octave for efficient system level simulation', *Numerical Algorithms* 87, 1729–1748.
- Roberts, A. J., MacKenzie, T. & Bunder, J. (2014), 'A dynamical systems approach to simulating macroscale spatial dynamics in multiple dimensions', *J. Engineering Mathematics* 86(1), 175–207.

http://arxiv.org/abs/1103.1187