

Equation-Free function toolbox for Matlab/Octave: Full Developers Manual

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Abstract

This ‘equation-free toolbox’ empowers the computer-assisted analysis of complex, multiscale systems. Its aim is to enable you to use microscopic simulators to perform system level tasks and analysis, because microscale simulations are often the best available description of a system. The methodology bypasses the derivation of macroscopic evolution equations by computing only short bursts of the microscale simulator (Kevrekidis & Samaey 2009, Kevrekidis et al. 2004, 2003, e.g.), and often only computing on small patches of the spatial domain (Roberts et al. 2014, e.g.). This suite of functions empowers users to start implementing such methods in their own applications. Download via <https://github.com/uoa1184615/EquationFreeGit>

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1 Introduction

This Developers Manual contains complete descriptions of the code in each function in the toolbox, and of each example. For concise descriptions of each function, quick start guides, and some basic examples, see the User Manual.

Users Download via <https://github.com/uaa1184615/EquationFreeGit>. Place the folder of this toolbox in a path searched by MATLAB/Octave. Then read the section(s) that documents the function of interest.

Quick start Maybe start by adapting one of the included examples. Many of the main functions include, at their beginning, example code of their use—code which is executed when the function is invoked without any arguments.

- To projectively integrate over time a multiscale, slow-fast, system of ODEs you could use `PIRK2()`, or `PIRK4()` for higher-order accuracy: adapt the Michaelis–Menten example at the beginning of `PIRK2.m` ([Section 2.2.2](#)).
- You may use forward bursts of simulation in order to simulate the slow dynamics backward in time, as in `egPIMM.m` ([Section 2.3](#)).
- To only resolve the slow dynamics in the projective integration, use lifting and restriction functions by adapting the singular perturbation ODE example at the beginning of `PIG.m` ([Section 2.4.2](#)).

Space-time systems Consider an evolving system over a large spatial domain when all you have is a microscale code. To efficiently simulate over the large domain, one can simulate in just small patches of the domain, appropriately coupled.

- In 1D space adapt the code at the beginning of `configPatches1.m` for Burgers' PDE ([Section 3.1.1](#)), or the staggered patches of 1D water wave equations in `waterWaveExample.m` ([Section 3.7](#)).
- In 2D space adapt the code at the beginning of `configPatches2.m` for nonlinear diffusion ([Section 4.1.1](#)), or the regular patches of the 2D wave PDE of `wave2D.m` ([Section 4.4](#)).
- In 3D space adapt the code at the beginning of `configPatches3.m` for wave propagation through a heterogeneous medium ([Section 5.1.1](#)), or the patches of the 3D heterogeneous diffusion of `homoDiffEdgy3.m` ([Section 5.4](#)).
- Other provided examples include cases of macroscale *computational homogenisation* of microscale heterogeneity.

- In MATLAB, the axis labelling works best if one executes
`set(groot,'defaultTextInterpreter','latex')`

Verification Most of these schemes have proven ‘accuracy’ when compared to the underlying specified microscale system. In the spatial patch schemes, we measure ‘accuracy’ by the order of consistency between macroscale dynamics and the specified microscale.

- [Roberts & Kevrekidis \(2007\)](#) and [Roberts et al. \(2014\)](#) proved reasonably general high-order consistency for the 1D and 2D patch schemes, respectively.
- In wave-like systems, [Cao & Roberts \(2016b\)](#) established high-order consistency for the 1D staggered patch scheme.
- A heterogeneous microscale is more difficult, but [Bunder et al. \(2017\)](#) showed good accuracy in a variety of circumstances, for appropriately chosen parameters. Further, [Bunder et al. \(2020\)](#) developed a new ‘edgy’ inter-patch interpolation that is proven to be good for simulating the macroscale homogenised dynamics of microscale heterogeneous systems—now coded in the toolbox.

Blackbox scenarios Suppose that you have a *detailed and trustworthy* computational simulation of some problem of interest. Let’s say the simulation is coded in terms of detailed (microscale) variable values $\vec{u}(t)$, in \mathbb{R}^p for some number p of field variables, and evolving in time t . The details \vec{u} could represent particles, agents, or states of a system. When the computation is too time consuming to simulate all the times of interest, then Projective Integration may be able to predict long-time dynamics, both forward and backward in time. In this case, provide your detailed computational simulation as a ‘black box’ to the Projective Integration functions of [Chapter 2](#).

In many scenarios, the problem of interest involves space or a ‘spatial’ lattice. Let’s say that indices i correspond to ‘spatial’ coordinates $\vec{x}_i(t)$, which are often fixed: in lattice problems the positions \vec{x}_i would be fixed in time (unless employing a moving mesh on the microscale); however, in particle problems the positions would evolve. And suppose your detailed and trustworthy simulation is coded also in terms of micro-field variable values $\vec{u}_i(t) \in \mathbb{R}^p$ at time t . Often the detailed computational simulation is too expensive over all the desired spatial domain $\vec{x} \in \mathbb{X} \subset \mathbb{R}^d$. In this case, the toolbox functions of [Chapter 3](#) empower you to simulate on only small, well-separated, patches of space by appropriately coupling between patches your simulation code, as a ‘black box’, executing on each small patch. The computational savings may be enormous, especially if combined with projective integration.

[Chapter 6](#) provides small examples of how to parallelise the patch computations over multiple processors. But such parallelisation may be only useful for scenarios where the microscale code has many millions of operations per time-step.

Contributors The aim of this project is to collectively develop a MATLAB/Octave toolbox of equation-free algorithms. Initially the algorithms are basic, and the plan is to subsequently develop more and more capability.

MATLAB appears a good choice for a first version since it is widespread, efficient, supports various parallel modes, and development costs are reasonably low. Further it is built on BLAS and LAPACK so the cache and superscalar CPU are potentially well utilised. We aim to develop functions that work for MATLAB/Octave. [Appendix A](#) outlines some details for contributors.

2 Projective integration of deterministic ODEs

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2.1 Introduction

This section provides some good projective integration functions ([Gear & Kevrekidis 2003b,c](#), [Givon et al. 2006](#), [Marschler et al. 2014](#), [Maclean & Gottwald 2015](#), [Sieber et al. 2018](#), e.g.). The goal is to enable computationally expensive multiscale dynamic simulations/integrations to efficiently compute over very long time scales.

Quick start [Section 2.2.2](#) shows the most basic use of a projective integration function. [Section 2.3](#) shows how to code more variations of the introductory example of a long time simulation of the Michaelis–Menton multiscale system of differential equations. Then see [Figures 2.1](#) and [2.2](#)

Scenario When you are interested in a complex system with many interacting parts or agents, you usually are primarily interested in the self-organised emergent macroscale characteristics. Projective integration empowers us to efficiently simulate such long-time emergent dynamics. We suppose you have coded some accurate, fine-scale, microscale simulation of the complex system, and call such code a microsolver.

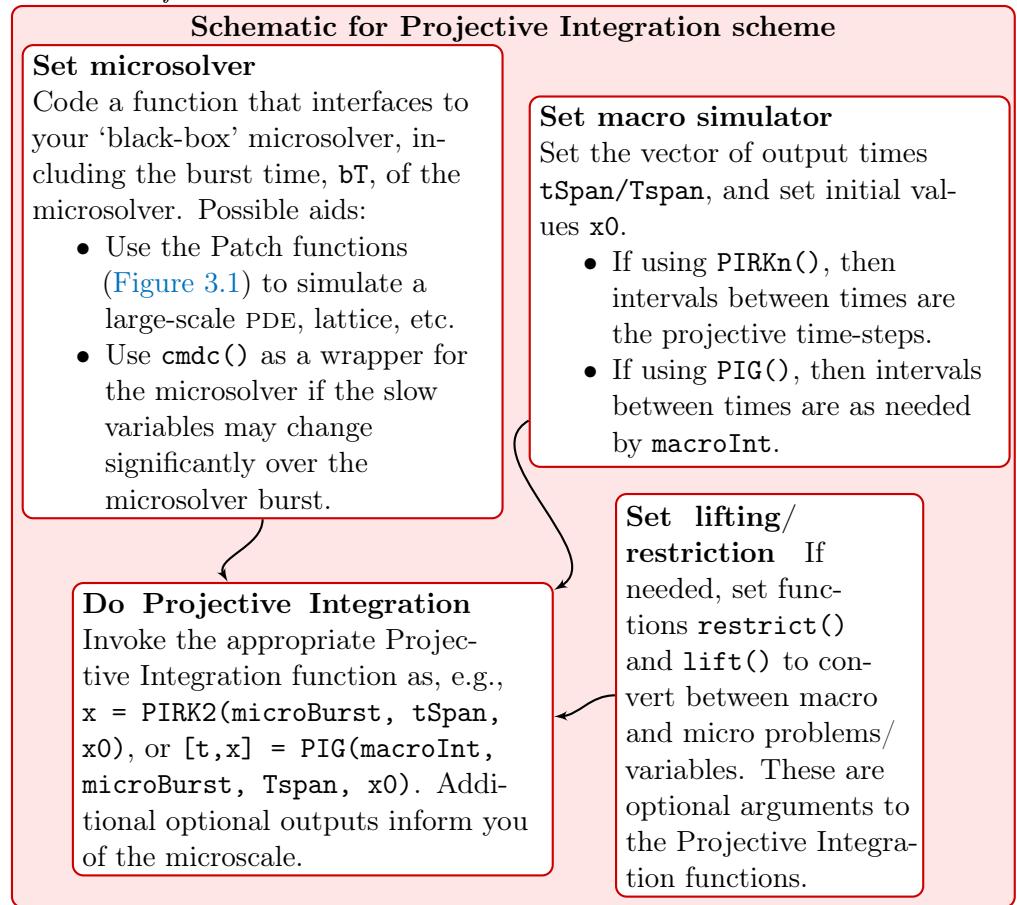
The Projective Integration section of this toolbox consists of several functions. Each function implements over a long-time scale a variant of a standard numerical method to simulate/integrate the emergent dynamics of the complex system. Each function has standardised inputs and outputs.

[Petersik \(2019–\)](#) is also developing, in python, some projective integration functions.

Main functions

- Projective Integration by second or fourth-order Runge–Kutta is implemented by `PIRK2()` or `PIRK4()` respectively. These schemes are suitable for precise simulation of the slow dynamics, provided the time period spanned by an application of the microsolver is not too large.
- Projective Integration with a General method, `PIG()`. This function enables a Projective Integration implementation of any integration method over macroscale time-steps. It does not matter whether the method is a standard MATLAB/Octave algorithm, or one supplied by the user. `PIG()` should only be used directly in very stiff systems, less stiff systems additionally require `cdmc()`.
- *Constraint-defined manifold computing*, `cdmc()`, is a helper function, based on the method introduced in [Gear et al. \(2005a\)](#), that iteratively applies the microsolver and backward projection in time. The result is to project the fast variables close to the slow manifold, without advancing the current time by the burst time of the microsolver. This function reduces errors related to the simulation length of the microsolver in the `PIG` function. In particular, it enables `PIG()` to be used on problems that are not particularly stiff.

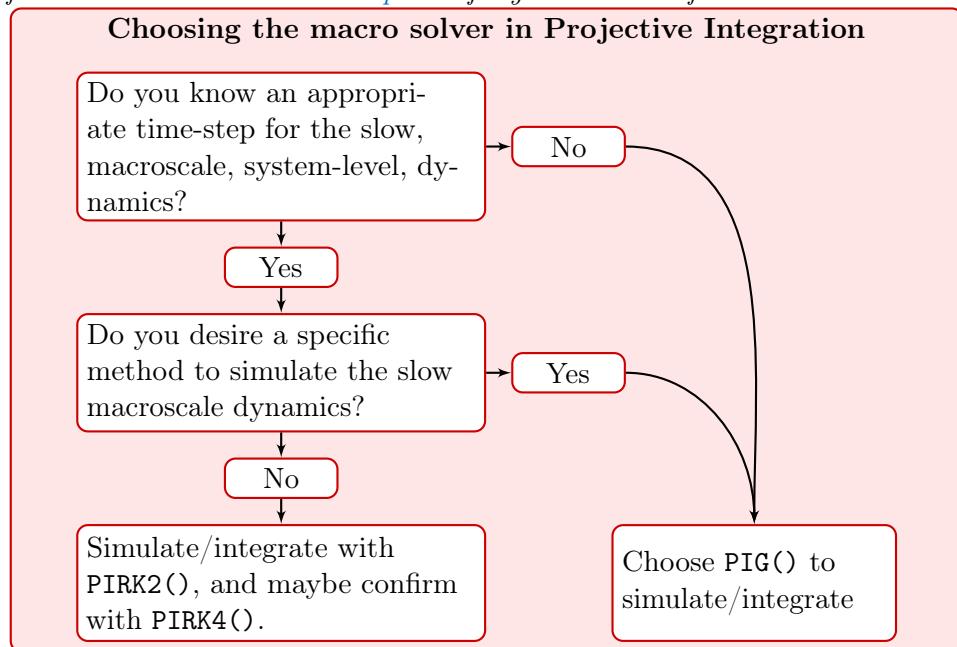
Figure 2.1: The Projective Integration method greatly accelerates simulation/integration of a system exhibiting multiple time scales. The Projective Integration Chapter 2 presents several separate functions, as well as several optional wrapper functions that may be invoked. This chart overviews constructing a Projective Integration simulation, whereas Figure 2.2 roughly guides which top-level Projective Integration functions should be used. Chapter 2 fully details each function.



The above functions share dependence on a user-specified *microsolver* that accurately simulates some problem of interest.

The following sections describe the `PIRK2()` and `PIG()` functions in detail, providing an example for each. The function `PIRK4()` is very similar to `PIRK2()`. Descriptions for the minor functions follow, and an example using `cdmc()`.

Figure 2.2: The Projective Integration method greatly accelerates simulation/integration of a system exhibiting multiple time scales. In conjunction with [Figure 2.1](#), this chart roughly guides which top-level Projective Integration functions should be used. [Chapter 2](#) fully details each function.



2.2 PIRK2(): projective integration of second-order accuracy

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2.2.1 Introduction

This Projective Integration scheme implements a macroscale scheme that is analogous to the second-order Runge–Kutta Improved Euler integration.

```
21 function [x, tms, xms, rm, svf] = PIRK2(microBurst, tSpan, x0, bT)
```

Input If there are no input arguments, then this function applies itself to the Michaelis–Menton example: see the code in [Section 2.2.2](#) as a basic template of how to use.

- `microBurst()`, a user-coded function that computes a short-time burst of the microscale simulation.

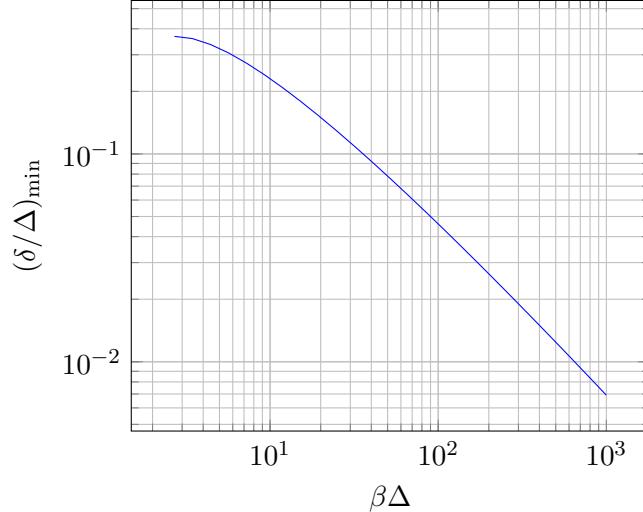
```
[tOut, xOut] = microBurst(tStart, xStart, bT)
```

- Inputs: `tStart`, the start time of a burst of simulation; `xStart`, the row n -vector of the starting state; `bT`, *optional*, the total time to simulate in the burst—if your `microBurst()` determines the burst time, then replace `bT` in the argument list by `varargin`.
- Outputs: `tOut`, the column vector of solution times; and `xOut`, an array in which each *row* contains the system state at corresponding times.

Be wary that for very large scale separations (such as `MMepsilon<1e-5` in the Michaelis–Menton example), microscale integration by error-controlled variable-step routines (such as `ode23/45`) often generate microscale variations that ruin the projective extrapolation of `PIRK2()`. In such cases, a fixed time-step microscale integrator is much better (such as `rk2Int()`).

- `tSpan` is an ℓ -vector of times at which the user requests output, of which the first element is always the initial time. `PIRK2()` does not use adaptive time-stepping; the macroscale time-steps are (nearly) the steps between elements of `tSpan`.
- `x0` is an n -vector of initial values at the initial time `tSpan(1)`. Elements of `x0` may be `Nan`: such `Nans` are carried in the simulation through to the output, and often represent boundaries/edges in spatial fields.

Figure 2.3: Need macroscale step Δ such that $|\alpha\Delta| \lesssim \sqrt{6\varepsilon}$ for given relative error ε and slow rate α , and then $\delta/\Delta \gtrsim \frac{1}{\beta\Delta} \log |\beta\Delta|$ determines the minimum required burst length δ for every given fast rate β .



- bT , optional, either missing, or empty (`[]`), or a scalar: if a given scalar, then it is the length of the micro-burst simulations—the minimum amount of time needed for the microscale simulation to relax to the slow manifold; else if missing or `[]`, then `microBurst()` must itself determine the length of a burst.

```
77 if nargin<4, bT=[]; end
```

Choose a long enough burst length Suppose: firstly, you have some desired relative accuracy ε that you wish to achieve (e.g., $\varepsilon \approx 0.01$ for two digit accuracy); secondly, the slow dynamics of your system occurs at rate/frequency of magnitude about α ; and thirdly, the rate of *decay* of your fast modes are faster than the lower bound β (e.g., if three fast modes decay roughly like $e^{-12t}, e^{-34t}, e^{-56t}$ then $\beta \approx 12$). Then set

1. a macroscale time-step, $\Delta = \text{diff}(tSpan)$, such that $\alpha\Delta \approx \sqrt{6\varepsilon}$, and
2. a microscale burst length, $\delta = bT \gtrsim \frac{1}{\beta} \log |\beta\Delta|$, see Figure 2.3.

Output If there are no output arguments specified, then a plot is drawn of the computed solution x versus `tSpan`.

- x , an $\ell \times n$ array of the approximate solution vector. Each row is an estimated state at the corresponding time in `tSpan`. The simplest usage is then `x = PIRK2(microBurst,tSpan,x0,bT)`.

However, microscale details of the underlying Projective Integration computations may be helpful. `PIRK2()` provides up to four optional outputs of the microscale bursts.

- tms , optional, is an L dimensional column vector containing the microscale times within the burst simulations, each burst separated by `NaN`;

- **xms**, optional, is an $L \times n$ array of the corresponding microscale states—each rows is an accurate estimate of the state at the corresponding time **tms** and helps visualise details of the solution.
- **rm**, optional, a struct containing the ‘remaining’ applications of the microBurst required by the Projective Integration method during the calculation of the macrostep:
 - **rm.t** is a column vector of microscale times; and
 - **rm.x** is the array of corresponding burst states.

The states **rm.x** do not have the same physical interpretation as those in **xms**; the **rm.x** are required in order to estimate the slow vector field during the calculation of the Runge–Kutta increments, and do *not* accurately approximate the macroscale dynamics.

- **svf**, optional, a struct containing the Projective Integration estimates of the slow vector field.
 - **svf.t** is a 2ℓ dimensional column vector containing all times at which the Projective Integration scheme is extrapolated along microBurst data to form a macrostep.
 - **svf.dx** is a $2\ell \times n$ array containing the estimated slow vector field.

2.2.2 If no arguments, then execute an example

```
182 if nargin==0
```

Example code for Michaelis–Menton dynamics The Michaelis–Menton enzyme kinetics is expressed as a singularly perturbed system of differential equations for $x(t)$ and $y(t)$:

$$\frac{dx}{dt} = -x + (x + \frac{1}{2})y \quad \text{and} \quad \frac{dy}{dt} = \frac{1}{\epsilon} [x - (x + 1)y]$$

(encoded in function **MMburst()** in the next paragraph). With initial conditions $x(0) = 1$ and $y(0) = 0$, the following code computes and plots a solution over time $0 \leq t \leq 6$ for parameter $\epsilon = 0.05$. Since the rate of decay is $\beta \approx 1/\epsilon$ we choose a burst length $\epsilon \log(\Delta/\epsilon)$ as here the macroscale time-step $\Delta = 1$.

```
203 global MMepsilon
204 MMepsilon = 0.05
205 ts = 0:6
206 bT = MMepsilon*log( (ts(2)-ts(1))/MMepsilon )
207 [x,tms,xms] = PIRK2(@MMburst, ts, [1;0], bT);
208 figure, plot(ts,x,'o:',tms,xms)
209 title('Projective integration of Michaelis--Menton enzyme kinetics')
210 xlabel('time t'), legend('x(t)', 'y(t)')
```

Upon finishing execution of the example, exit this function.

```
216 return
217 end%if no arguments
```

Code a burst of Michaelis–Menten enzyme kinetics Integrate a burst of length bT of the ODEs for the Michaelis–Menten enzyme kinetics at parameter ϵ inherited from above. Code ODEs in function `dMMdt` with variables $x = \mathbf{x}(1)$ and $y = \mathbf{x}(2)$. Starting at time ti , and state xi (row), we here simply use MATLAB/Octave's `ode23/lsode` to integrate a burst in time.

```

15 function [ts, xs] = MMburst(ti, xi, bT)
16     global MMepsilon
17     dMMdt = @(t,x) [ -x(1)+(x(1)+0.5)*x(2)
18                      1/MMepsilon*( x(1)-(x(1)+1)*x(2) ) ];
19     if ~exist('OCTAVE_VERSION','builtin')
20         [ts, xs] = ode23(dMMdt, [ti ti+bT], xi);
21     else % octave version
22         [ts, xs] = odeOct(dMMdt, [ti ti+bT], xi);
23     end
24 end
25
26 function [ts, xs] = odeOct(dxdt,tSpan,x0)
27     if length(tSpan)>2, ts = tSpan;
28     else ts = linspace(tSpan(1),tSpan(end),21);
29     end
30     % mimic ode45 and ode23, but much slower for non-PI
31     lsode_options('integration method','non-stiff');
32     xs = lsode(@(x,t) dxdt(t,x),x0,ts);
33 end

```

2.2.3 The projective integration code

Determine the number of time-steps and preallocate storage for macroscale estimates.

```

236 nT=length(tSpan);
237 x=nan(nT,length(x0));

```

Get the number of expected outputs and set logical indices to flag what data should be saved.

```

245 nArgOut=nargout();
246 saveMicro = (nArgOut>1);
247 saveFullMicro = (nArgOut>3);
248 saveSvf = (nArgOut>4);

```

Run a preliminary application of the microBurst on the given initial state to help relax to the slow manifold. This is done in addition to the microBurst in the main loop, because the initial state is often far from the attracting slow manifold. Require the user to input and output rows of the system state.

```

261 x0 = reshape(x0,1,[]);
262 [relax_t,relax_x0] = microBurst(tSpan(1),x0,bT);

```

Use the end point of this preliminary microBurst as the initial state for the loop of macro-steps.

```

270 tSpan(1) = relax_t(end);
271 x(1,:)=relax_x0(end,:);
```

If saving information, then record the first application of the microBurst. Allocate cell arrays for times and states for outputs requested by the user, as concatenating cells is much faster than iteratively extending arrays.

```

281 if saveMicro
282     tms = cell(nT,1);
283     xms = cell(nT,1);
284     tms{1} = reshape(relax_t,[],1);
285     xms{1} = relax_x0;
286     if saveFullMicro
287         rm.t = cell(nT,1);
288         rm.x = cell(nT,1);
289         if saveSvf
290             svf.t = nan(2*nT-2,1);
291             svf.dx = nan(2*nT-2,length(x0));
292         end
293     end
294 end
```

Loop over the macroscale time-steps Also set an initial rounding tolerance for checking.

```

303 roundingTol = 1e-8;
304 for jT = 2:nT
305     T = tSpan(jT-1);
```

If two applications of the microBurst would cover one entire macroscale time-step, then do so (setting some internal states to NaN); else proceed to projective step.

```

313     if ~isempty(bT) && 2*abs(bT)>=abs(tSpan(jT)-T) && bT*(tSpan(jT)-T)>0
314         [t1,xm1] = microBurst(T, x(jT-1,:), tSpan(jT)-T);
315         x(jT,:) = xm1(end,:);
316         t2 = nan;    xm2 = nan(1,size(xm1,2));
317         dx1 = xm2;  dx2 = xm2;
318     else
```

Run the first application of the microBurst; since this application directly follows from the initial conditions, or from the latest macrostep, this macroscale information is physically meaningful as a simulation of the system. Extract the size of the final time-step.

```
329 [t1,xm1] = microBurst(T, x(jT-1,:), bT);
```

To estimate the derivative by numerical differentiation, we balance approximation error $\|\ddot{x}\|/dt$ with round-off error $\|x\|\epsilon/dt$ by the optimal time-step $dt \approx \sqrt{(\|x\|\epsilon/\|\ddot{x}\|)}$. Omit $\|\ddot{x}\|$ as we do not know it. Also, limit dt to at most the last tenth of the burst, and at least one step.

```

341     nt = length(t1);
342     optdt = min(0.1*(t1(nt)-t1(1)),sqrt(max(rms(xm1))*1e-15));
343     [~,kt] = min(abs(t1(nt)-optdt-t1(1:nt-1)));
344     ktnt = [kt nt];
345     del = t1(nt)-t1(kt);

```

Check for round-off error, and decrease tolerance so that warnings are not repeated unless things get worse.

```

352     xt = [reshape(t1(ktnt),[],1) xm1(ktnt,:)];
353     if norm(diff(xt))/norm(xt,'fro') < roundingTol
354         warning(['significant round-off error in 1st projection at T=' num2str(T)])
355         roundingTol = roundingTol/10;
356     end

```

Find the needed time-step to reach time $tSpan(n+1)$ and form a first estimate $dx1$ of the slow vector field.

```

365     Dt = tSpan(jT)-t1(end);
366     dx1 = (xm1(nt,:)-xm1(kt,:))/del;

```

Project along $dx1$ to form an intermediate approximation of x ; run another application of the microBurst and form a second estimate of the slow vector field (assuming the burst length is the same, or nearly so).

```

376     xint = xm1(end,:)+(Dt-(t1(end)-t1(1)))*dx1;
377     [t2,xm2] = microBurst(T+Dt, xint, bT);

```

As before, choose dt as best we can to estimate derivative.

```

384     nt = length(t2);
385     optdt = min(0.1*(t2(nt)-t2(1)),sqrt(max(rms(xm2))*1e-15));
386     [~,kt] = min(abs(t2(nt)-optdt-t2(1:nt-1)));
387     ktnt = [kt nt];
388     del = t2(nt)-t2(kt);
389     dx2 = (xm2(nt,:)-xm2(kt,:))/del;

```

Check for round-off error, and decrease tolerance so that warnings are not repeated unless things get worse.

```

396     xt = [reshape(t2(ktnt),[],1) xm2(ktnt,:)];
397     if norm(diff(xt))/norm(xt,'fro') < roundingTol
398         warning(['significant round-off error in 2nd projection at T=' num2str(T)])
399         roundingTol = roundingTol/10;
400     end

```

Use the weighted average of the estimates of the slow vector field to take a macro-step.

```

408     x(jT,:) = xm1(end,:)+Dt*(dx1+dx2)/2;

```

Now end the if-statement that tests whether a projective step saves simulation time.

```

416     end

```

If saving trusted microscale data, then populate the cell arrays for the current loop iterate with the time-steps and output of the first application of the microBurst. Separate bursts by NaNs.

```
426     if saveMicro
427         tms{jT} = [reshape(t1,[],1); nan];
428         xms{jT} = [xm1; nan(1,size(xm1,2))];
```

If saving all microscale data, then repeat for the remaining applications of the microBurst.

```
436     if saveFullMicro
437         rm.t{jT} = [reshape(t2,[],1); nan];
438         rm.x{jT} = [xm2; nan(1,size(xm2,2))];
```

If saving Projective Integration estimates of the slow vector field, then populate the corresponding cells with times and estimates.

```
447     if saveSvf
448         svf.t(2*jT-3:2*jT-2) = [t1(end); t2(end)];
449         svf.dx(2*jT-3:2*jT-2,:) = [dx1; dx2];
450     end
451 end
452 end
```

End the main loop over all the macro-steps.

```
458 end
Overwrite x(1,:) with the specified initial condition tSpan(1).
467 x(1,:) = reshape(x0,1,[]);
```

For additional requested output, concatenate all the cells of time and state data into two arrays.

```
475 if saveMicro
476     tms = cell2mat(tms);
477     xms = cell2mat(xms);
478     if saveFullMicro
479         rm.t = cell2mat(rm.t);
480         rm.x = cell2mat(rm.x);
481     end
482 end
```

2.2.4 If no output specified, then plot the simulation

```
490 if nArgOut==0
491     figure, plot(tSpan,x,'o:')
492     title('Projective Simulation with PIRK2')
493 end
```

This concludes PIRK2().

```
500 end
```

2.3 egPIMM: Example projective integration of Michaelis–Menton kinetics

The Michaelis–Menton enzyme kinetics is expressed as a singularly perturbed system of differential equations for $x(t)$ and $y(t)$:

$$\frac{dx}{dt} = -x + (x + \frac{1}{2})y \quad \text{and} \quad \frac{dy}{dt} = \frac{1}{\epsilon} [x - (x + 1)y]$$

(encoded in function `MMburst()` below). As illustrated by [Figure 2.5](#), the slow variable $x(t)$ evolves on a time scale of one, whereas the fast variable $y(t)$ evolves on a time scale of the small parameter ϵ .

Invoke projective integration Clear, and set the scale separation parameter ϵ to something small like 0.01. Here use $\epsilon = 0.1$ for clearer graphs.

```
31 clear all, close all
32 global MMepsilon
33 MMepsilon = 0.1
```

First, the end of this section encodes the computation of bursts of the Michaelis–Menton system in a function `MMburst()`. Second, here set macroscale times of computation and interest into vector `ts`. Then, invoke Projective Integration with `PIRK2()` applied to the burst function, say using bursts of simulations of length 2ϵ , and starting from the initial condition for the Michaelis–Menton system, at time $t = 0$, of $(x, y) = (1, 0)$ (off the slow manifold).

```
48 ts = 0:6
49 xs = PIRK2(@MMburst, ts, [1;0], 2*MMepsilon)
50 plot(ts,xs,'o:')
51 xlabel('time t'), legend('x(t)', 'y(t)')
52 title('macroscale points only')
53 ifOurCf2eps([mfilename '1'])
54 pause(1)
```

[Figure 2.4](#) plots the macroscale results showing the long time decay of the Michaelis–Menton system on the slow manifold. [Sieber et al. \(2018\)](#) [§4] used this system as an example of their analysis of the convergence of Projective Integration.

Request and plot the microscale bursts Because the initial conditions of the simulation are off the slow manifold, the initial macroscale step appears to ‘jump’ ([Figure 2.4](#)). In order to see the initial transient attraction to the slow manifold we plot some microscale data in [Figure 2.5](#). Two further output variables provide this microscale burst information.

```
80 [xs,tMicro,xMicro] = PIRK2(@MMburst, ts, [1;0], 2*MMepsilon);
81 figure, plot(ts,xs,'o:',tMicro,xMicro)
82 xlabel('time t'), legend('x(t)', 'y(t)')
83 title('macroscale points with microscale bursts')
84 ifOurCf2eps([mfilename '2'])
85 pause(1)
```

Figure 2.4: Michaelis–Menten enzyme kinetics simulated with the projective integration of PIRK2(): macroscale samples.

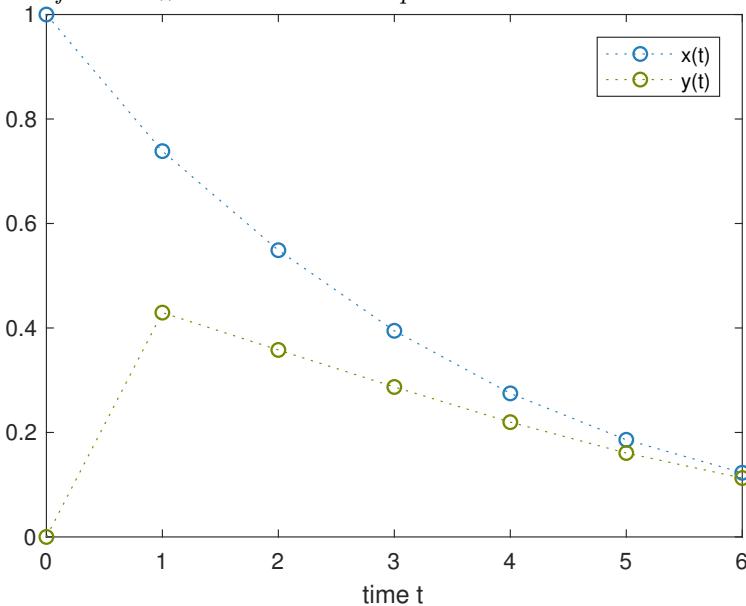


Figure 2.5 plots the macroscale and microscale results—also showing that the initial burst is by default twice as long. Observe the slow variable $x(t)$ is also affected by the initial transient (hence other schemes which ‘freeze’ slow variables are less accurate).

Simulate backward in time Figure 2.6 shows that projective integration even simulates backward in time along the slow manifold using short forward bursts (Gear & Kevrekidis 2003a, Frewen et al. 2009). Such backward macroscale simulations succeed despite the fast variable $y(t)$, when backward in time, being viciously unstable. However, backward integration appears to need longer bursts, here 3ϵ .

```

115 ts = 0:-1:-5
116 [xs,tMicro,xMicro] = PIRK2(@MMburst, ts, 0.2*[1;1], 3*MMepsilon);
117 figure, plot(ts, xs, 'o:', tMicro, xMicro)
118 xlabel('time t'), legend('x(t)', 'y(t)')
119 title('backward integration showing points with bursts')
120 ifOurCf2eps([mfilename '3'])

```

Code a burst of Michaelis–Menten enzyme kinetics Integrate a burst of length bT of the ODEs for the Michaelis–Menten enzyme kinetics at parameter ϵ inherited from above. Code ODEs in function `dMMdt` with variables $x = \mathbf{x}(1)$ and $y = \mathbf{x}(2)$. Starting at time `ti`, and state `xi` (row), we here simply use MATLAB/Octave’s `ode23/lsode` to integrate a burst in time.

```

15 function [ts, xs] = MMburst(ti, xi, bT)
16     global MMepsilon
17     dMMdt = @(t,x) [-x(1)+(x(1)+0.5)*x(2)
18                      1/MMepsilon*( x(1)-(x(1)+1)*x(2) )];

```

Figure 2.5: Michaelis–Menten enzyme kinetics simulated with the projective integration of PIRK2(): the microscale bursts show the initial transients on a time scale of $\epsilon = 0.1$, and then the alignment along the slow manifold.

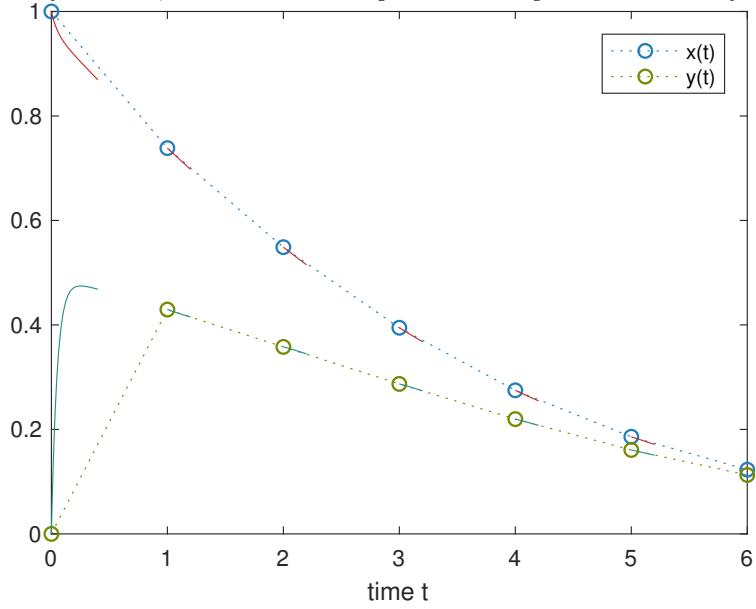
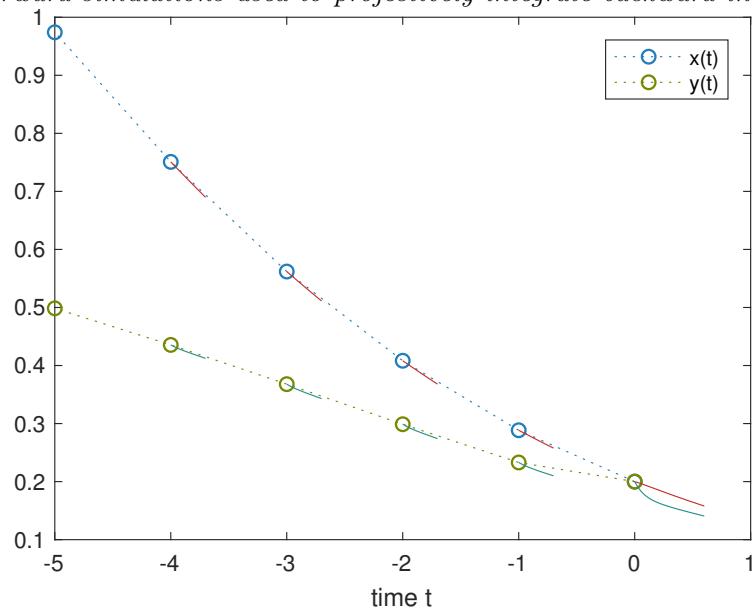


Figure 2.6: Michaelis–Menten enzyme kinetics at $\epsilon = 0.1$ simulated backward with the projective integration of PIRK2(): the microscale bursts show the short forward simulations used to projectively integrate backward in time.



```
19      if ~exist('OCTAVE_VERSION','builtin')
20      [ts, xs] = ode23(dMMdt, [ti ti+bT], xi);
21      else % octave version
22      [ts, xs] = odeOct(dMMdt, [ti ti+bT], xi);
23      end
24  end

8  function [ts,xs] = odeOct(dxdt,tSpan,x0)
9      if length(tSpan)>2, ts = tSpan;
10     else ts = linspace(tSpan(1),tSpan(end),21);
11     end
12     % mimic ode45 and ode23, but much slower for non-PI
13     lsode_options('integration method','non-stiff');
14     xs = lsode(@(x,t) dxdt(t,x),x0,ts);
15  end
```

2.4 PIG(): Projective Integration via a General macroscale integrator

Section contents

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2.4.1 Introduction

This is a Projective Integration scheme when the macroscale integrator is any specified coded method. The advantage is that one may use MATLAB/Octave's inbuilt integration functions, with all their sophisticated error control and adaptive time-stepping, to do the macroscale integration/simulation.

By default, for the microscale simulations `PIG()` uses ‘constraint-defined manifold computing’, `cdmc()` ([Section 2.6](#)). This algorithm, initiated by [Gear et al. \(2005b\)](#), uses a backward projection so that the simulation time is unchanged after running the microscale simulator.

```
30 function [T,X,tms,xms,svf] = PIG(macroInt,microBurst,Tspan,x0 ...
31 ,restrict,lift,cdmcFlag)
```

Inputs:

- `macroInt()`, the numerical method that the user wants to apply on a slow-time macroscale. Either specify a standard MATLAB/Octave integration function (such as '`ode23`' or '`ode45`'), or code your own integration function using standard arguments. That is, if you code your own, then it must be

$$[Ts, Xs] = \text{macroInt}(F, Tspan, X0)$$

where

- function $F(T, X)$ notionally evaluates the time derivatives $d\vec{X}/dt$ at any time;
- $Tspan$ is either the macro-time interval, or the vector of macroscale times at which macroscale values are to be returned; and
- $X0$ are the initial values of \vec{X} at time $Tspan(1)$.

Then the i th *row* of Xs , $Xs(i,:)$, is to be the vector $\vec{X}(t)$ at time $t = Ts(i)$. Remember that in `PIG()` the function $F(T, X)$ is to be estimated by Projective Integration.

- `microBurst()` is a function that produces output from the user-specified code for a burst of microscale simulation. The function must internally specify/decide how long a burst it is to use. Usage

```
[tbs,xbs] = microBurst(tb0,xb0)
```

Inputs: `tb0` is the start time of a burst; `xb0` is the n -vector microscale state at the start of a burst.

Outputs: `tbs`, the vector of solution times; and `xbs`, the corresponding microscale states.

- `Tspan`, a vector of macroscale times at which the user requests output. The first element is always the initial time. If `macroInt` reports adaptively selected time steps (e.g., `ode45`), then `Tspan` consists of an initial and final time only.
- `x0`, the n -vector of initial microscale values at the initial time `Tspan(1)`.

Optional Inputs: `PIG()` allows for none, two or three additional inputs after `x0`. If you distinguish distinct microscale and macroscale states and your aim is to do Projective Integration on the macroscale only, then lifting and restriction functions must be provided to convert between them. Usage `PIG(...,restrict,lift)`:

- `restrict(x)`, a function that takes an input high-dimensional, n -D, microscale state \vec{x} and computes the corresponding low-dimensional, N -D, macroscale state \vec{X} ;
- `lift(X,xApprox)`, a function that converts an input low-dimensional, N -D, macroscale state \vec{X} to a corresponding high-dimensional, n -D, microscale state \vec{x} , given that `xApprox` is a recently computed microscale state on the slow manifold.

Either both `restrict()` and `lift()` are to be defined, or neither. If neither are defined, then they are assumed to be identity functions, so that `N=n` in the following.

If desired, the default constraint-defined manifold computing microsolver may be disabled, via `PIG(...,restrict,lift,cdmcFlag)`

- `cdmcFlag`, *any* seventh input to `PIG()`, will disable `cdmc()`, e.g., the string '`cdmc off`'.

If the `cdmcFlag` is to be set without using a `restrict()` or `lift()` function, then use empty matrices [] for the restrict and lift functions.

Output Between zero and five outputs may be requested. If there are no output arguments specified, then a plot is drawn of the computed solution `X` versus `T`. Most often you would store the first two output results of `PIG()`, via say `[T,X] = PIG(...)`.

- `T`, an L -vector of times at which `macroInt` produced results.

- \mathbf{X} , an $L \times N$ array of the computed solution: the i th row of \mathbf{X} , $\mathbf{X}(i, :)$, is to be the macro-state vector $\vec{X}(t)$ at time $t = T(i)$.

However, microscale details of the underlying Projective Integration computations may be helpful, and so `PIG()` provides some optional outputs of the microscale bursts, via `[T,X,tms,xms] = PIG(...)`

- \mathbf{tms} , optional, is an ℓ -dimensional column vector containing microscale times with bursts, each burst separated by `NaN`;
- \mathbf{xms} , optional, is an $\ell \times n$ array of the corresponding microscale states.

In some contexts it may be helpful to see directly how Projective Integration approximates a reduced slow vector field, via `[T,X,tms,xms,svf] = PIG(...)` in which

- \mathbf{svf} , optional, a struct containing the Projective Integration estimates of the slow vector field.
 - $\mathbf{svf}.T$ is a \hat{L} -dimensional column vector containing all times at which the microscale simulation data is extrapolated to form an estimate of $d\vec{x}/dt$ in `macroInt()`.
 - $\mathbf{svf}.dX$ is a $\hat{L} \times N$ array containing the estimated slow vector field.

If `macroInt()` is, for example, the forward Euler method (or the Runge–Kutta method), then $\hat{L} = L$ (or $\hat{L} = 4L$).

2.4.2 If no arguments, then execute an example

```
180 if nargin==0
```

As a basic example, consider a microscale system of the singularly perturbed system of differential equations

$$\frac{dx_1}{dt} = \cos(x_1) \sin(x_2) \cos(t) \quad \text{and} \quad \frac{dx_2}{dt} = \frac{1}{\epsilon} [\cos(x_1) - x_2]. \quad (2.1)$$

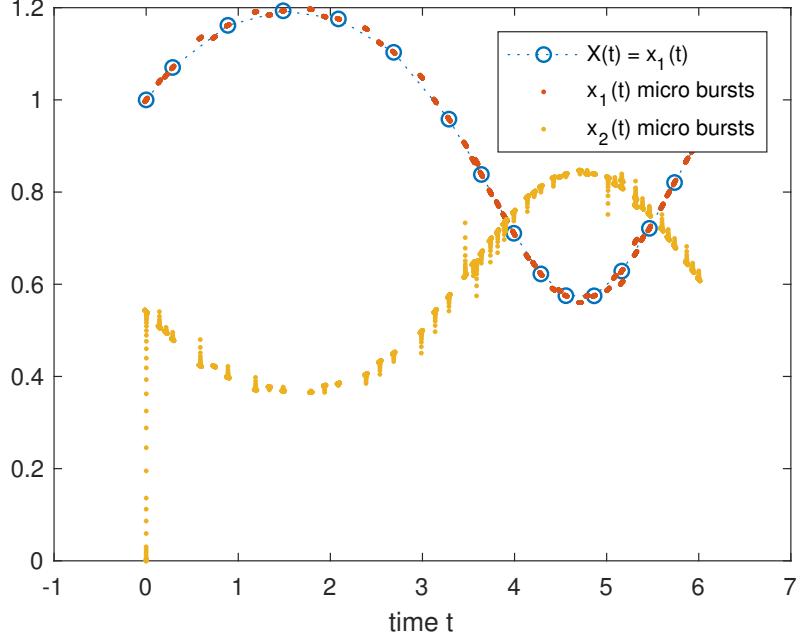
The macroscale variable is $X(t) = x_1(t)$, and the evolution dX/dt is unclear. With initial condition $X(0) = 1$, the following code computes and plots a solution of the system (2.1) over time $0 \leq t \leq 6$ for parameter $\epsilon = 10^{-3}$ (Figure 2.7). Whenever needed by `microBurst()`, the microscale system (2.1) is initialised ('lifted') using $x_2(t) = x_2^{\text{approx}}$ (yellow dots in Figure 2.7).

First we code the right-hand side function of the microscale system (2.1) of ODEs.

```
214 epsilon = 1e-3;
215 dxdt=@(t,x) [ cos(x(1))*sin(x(2))*cos(t)
216           ( cos(x(1))-x(2) )/epsilon ];
```

Second, we code microscale bursts, here using the standard `ode45()`. We choose a burst length $2\epsilon \log(1/\epsilon)$ as the rate of decay is $\beta \approx 1/\epsilon$ but we do not know the macroscale time-step invoked by `macroInt()`, so blithely assume $\Delta \leq 1$ and then double the usual formula for safety.

Figure 2.7: Projective Integration by PIG of the example system (2.1) with $\epsilon = 10^{-3}$ (Section 2.4.2). The macroscale solution $X(t)$ is represented by just the blue circles. The microscale bursts are the microscale states $(x_1(t), x_2(t)) = (\text{red}, \text{yellow})$ dots.



```

227 bT = 2*epsilon*log(1/epsilon)
228 if ~exist('OCTAVE_VERSION','builtin')
229     micB='ode45'; else micB='rk2Int'; end
230 microBurst = @(tb0, xb0) feval(micB,dxdt,[tb0 tb0+bT],xb0);

```

Third, code functions to convert between macroscale and microscale states.

```

237 restrict = @(x) x(1);
238 lift = @(X,xApprox) [X; xApprox(2)];

```

Fourth, invoke PIG to use MATLAB/Octave's `ode23/lsode`, say, on the macroscale slow evolution. Integrate the micro-bursts over $0 \leq t \leq 6$ from initial condition $\vec{x}(0) = (1, 0)$. You could set `Tspan=[0 -6]` to integrate backward in macroscale time with forward microscale bursts (Gear & Kevrekidis 2003a, Frewen et al. 2009).

```

250 Tspan = [0 6];
251 x0 = [1;0];
252 if ~exist('OCTAVE_VERSION','builtin')
253     macInt='ode23'; else macInt='odeOct'; end
254 [Ts,Xs,tms,xms] = PIG(macInt,microBurst,Tspan,x0,restrict,lift);

```

Plot output of this projective integration.

```

260 figure, plot(Ts,Xs,'o:',tms,xms,'.')
261 title('Projective integration of singularly perturbed ODE')
262 xlabel('time t')
263 legend('X(t) = x_1(t)', 'x_1(t) micro bursts', 'x_2(t) micro bursts')

```

Upon finishing execution of the example, exit this function.

```
269 return
270 end%if no arguments
```

2.4.3 The projective integration code

If no lifting/restriction functions are provided, then assign them to be the identity functions.

```
287 if nargin < 5 || isempty(restrict)
288     lift=@(X,xApprox) X;
289     restrict=@(x) x;
290 end
```

Get the number of expected outputs and set logical indices to flag what data should be saved.

```
298 nArgOut = nargin();
299 saveMicro = (nArgOut>2);
300 saveSvf = (nArgOut>4);
```

Find the number of time-steps at which output is expected, and the number of variables.

```
308 nT = length(Tspan)-1;
309 nx = length(x0);
310 nX = length(restrict(x0));
```

Reformulate the microsolver to use `cdmc()`, unless flagged otherwise. The result is that the solution from microBurst will terminate at the given initial time.

```
320 if nargin<7
321     microBurst = @(t,x) cdmc(microBurst,t,x);
322 else
323     warning(['A ' class(cdmFlag) ' seventh input to PIG()'...
324         ' PIG will not use constraint-defined manifold computing.'])
325 end
```

Execute a preliminary application of the microBurst on the initial state. This is done in addition to the microBurst in the main loop, because the initial state is often far from the attracting slow manifold.

```
337 [relaxT,x0MicroRelax] = microBurst(Tspan(1),x0);
338 xMicroLast = x0MicroRelax(end,:);
339 X0Relax = restrict(xMicroLast);
```

Update the initial time.

```
346 Tspan(1) = relaxT(end);
```

Allocate cell arrays for times and states for any of the outputs requested by the user. If saving information, then record the first application of the microBurst. It is unknown a priori how many applications of microBurst will

be required; this code may be run more efficiently if the correct number is used in place of $nT+1$ as the dimension of the cell arrays.

```

358 if saveMicro
359     tms=cell(nT+1,1); xms=cell(nT+1,1);
360     n=1;
361     tms{n} = reshape(relaxT,[],1);
362     xms{n} = x0MicroRelax;
363
364     if saveSvf
365         svf.T = cell(nT+1,1);
366         svf.dX = cell(nT+1,1);
367     else
368         svf = [];
369     end
370 else
371     tms = [] ; xms = [] ; svf = [] ;
372 end

```

Define a function of macro simulation The idea of `PIG()` is to use the output from the `microBurst()` to approximate an unknown function $F(t, X)$ that computes $d\vec{X}/dt$. This approximation is then used in the system/user-defined ‘coarse solver’ `macroInt()`. The approximation is computed in the function

```
385 function [dXdt]=PIFun(t,X)
```

Run a microBurst from the given macroscale initial values.

```

391 x = lift(X,xMicroLast);
392 [tTmp,xMicroTmp] = microBurst(t,reshape(x,[],1));
393 xMicroLast = xMicroTmp(end,:).';

```

Compute the standard Projective Integration approximation of the slow vector field.

```

400 X2 = restrict(xMicroTmp(end,:));
401 X1 = restrict(xMicroTmp(end-1,:));
402 dt = tTmp(end)-tTmp(end-1);
403 dXdt = (X2 - X1).'/dt;

```

Save the microscale data, and the Projective Integration slow vector field, if requested.

```

410 if saveMicro
411     n=n+1;
412     tms{n} = [reshape(tTmp,[],1); nan];
413     xms{n} = [xMicroTmp; nan(1,nx)];
414     if saveSvf
415         svf.T{n-1} = t;
416         svf.dX{n-1} = dXdt;
417     end

```

```

418     end
419 end% PIFun function

```

Invoke the macroscale integration Integrate PIF() with the user-specified simulator macroInt(). For some reason, in MATLAB/Octave we need to use a one-line function, PIF, that invokes the above macroscale function, PIFun. We also need to use feval because macroInt() has multiple outputs.

```

432 PIF = @(t,x) PIFun(t,x);
433 [T,X] = feval(macroInt,PIF,Tspan,X0Relax.');

```

Overwrite X(1,:) and T(1), which a user expects to be X0 and Tspan(1) respectively, with the given initial conditions.

```

442 X(1,:) = restrict(x0);
443 T(1) = Tspan(1);

```

Concatenate all the additional requested outputs into arrays.

```

450 if saveMicro
451     tms = cell2mat(tms);
452     xms = cell2mat(xms);
453     if saveSvf
454         svf.T = cell2mat(svf.T);
455         svf.dX = cell2mat(svf.dX);
456     end
457 end

```

2.4.4 If no output specified, then plot the simulation

```

465 if nArgOut==0
466     figure, plot(T,X,'o:')
467     title('Projective Simulation via PIG')
468 end

```

This concludes PIG().

```

476 end

```

2.5 PIRK4(): projective integration of fourth-order accuracy

Section contents

2.5.1	Introduction	30
2.5.2	The projective integration code	32
2.5.3	If no output specified, then plot the simulation	36

2.5.1 Introduction

This Projective Integration scheme implements a macrosolver analogous to the fourth-order Runge–Kutta method.

```
19 function [x, tms, xms, rm, svf] = PIRK4(microBurst, tSpan, x0, bT)
```

See [Section 2.2](#) as the inputs and outputs are the same as `PIRK2()`.

If no arguments, then execute an example

```
29 if nargin==0
```

Example of Michaelis–Menton backwards in time The Michaelis–Menton enzyme kinetics is expressed as a singularly perturbed system of differential equations for $x(t)$ and $y(t)$ (encoded in function `MMburst`):

$$\frac{dx}{dt} = -x + (x + \frac{1}{2})y \quad \text{and} \quad \frac{dy}{dt} = \frac{1}{\epsilon} [x - (x + 1)y].$$

With initial conditions $x(0) = y(0) = 0.2$, the following code uses forward time bursts in order to integrate backwards in time to $t = -5$ ([Frewen et al. 2009](#), e.g.). It plots the computed solution over time $-5 \leq t \leq 0$ for parameter $\epsilon = 0.1$. Since the rate of decay is $\beta \approx 1/\epsilon$ we choose a burst length $\epsilon \log(|\Delta|/\epsilon)$ as here the macroscale time-step $\Delta = -1$.

```
50 global MMepsilon
51 MMepsilon = 0.1
52 ts = 0:-1:-5
53 bT = MMepsilon*log(abs(ts(2)-ts(1))/MMepsilon)
54 [x,tms,xms,rm,svf] = PIRK4(@MMburst, ts, 0.2*[1;1], bT);
55 figure, plot(ts,x,'o:',tms,xms)
56 xlabel('time t'), legend('x(t)', 'y(t)')
57 title('Backwards-time projective integration of Michaelis--Menton')
58
59 % Plot the solution
60 plot(ts,x,'o:',tms,xms)
61 xlabel('time t'), legend('x(t)', 'y(t)')
62 title('Backwards-time projective integration of Michaelis--Menton')
63
64 end%if no arguments
```

Upon finishing execution of the example, exit this function.

Code a burst of Michaelis–Menten enzyme kinetics Integrate a burst of length bT of the ODEs for the Michaelis–Menten enzyme kinetics at parameter ϵ inherited from above. Code ODEs in function `dMMdt` with variables $x = \mathbf{x}(1)$ and $y = \mathbf{x}(2)$. Starting at time ti , and state xi (row), we here simply use MATLAB/Octave’s `ode23/lsode` to integrate a burst in time.

```

15 function [ts, xs] = MMburst(ti, xi, bT)
16     global MMepsilon
17     dMMdt = @(t,x) [ -x(1)+(x(1)+0.5)*x(2)
18                      1/MMepsilon*( x(1)-(x(1)+1)*x(2) ) ];
19     if ~exist('OCTAVE_VERSION','builtin')
20         [ts, xs] = ode23(dMMdt, [ti ti+bT], xi);
21     else % octave version
22         [ts, xs] = odeOct(dMMdt, [ti ti+bT], xi);
23     end
24 end
25
26 function [ts, xs] = odeOct(dxdt,tSpan,x0)
27     if length(tSpan)>2, ts = tSpan;
28     else ts = linspace(tSpan(1),tSpan(end),21);
29     end
30     % mimic ode45 and ode23, but much slower for non-PI
31     lsode_options('integration method','non-stiff');
32     xs = lsode(@(x,t) dxdt(t,x),x0,ts);
33 end

```

Input If there are no input arguments, then this function applies itself to the Michaelis–Menton example: see the code in [Section 2.2.2](#) as a basic template of how to use.

- `microBurst()`, a user-coded function that computes a short-time burst of the microscale simulation.

`[tOut, xOut] = microBurst(tStart, xStart, bT)`

- Inputs: `tStart`, the start time of a burst of simulation; `xStart`, the row n -vector of the starting state; `bT`, *optional*, the total time to simulate in the burst—if your `microBurst()` determines the burst time, then replace `bT` in the argument list by `varargin`.
- Outputs: `tOut`, the column vector of solution times; and `xOut`, an array in which each *row* contains the system state at corresponding times.

- `tSpan` is an ℓ -vector of times at which the user requests output, of which the first element is always the initial time. `PIRK4()` does not use adaptive time-stepping; the macroscale time-steps are (nearly) the steps between elements of `tSpan`.
- `x0` is an n -vector of initial values at the initial time `tSpan(1)`. Elements of `x0` may be `Nan`: such `Nans` are carried in the simulation through to the output, and often represent boundaries/edges in spatial fields.

- `bT`, optional, either missing, or empty (`[]`), or a scalar: if a given scalar, then it is the length of the micro-burst simulations—the minimum amount of time needed for the microscale simulation to relax to the slow manifold; else if missing or `[]`, then `microBurst()` must itself determine the length of a burst.

```
124 if nargin<4, bT=[]; end
```

Output If there are no output arguments specified, then a plot is drawn of the computed solution `x` versus `tSpan`.

- `x`, an $\ell \times n$ array of the approximate solution vector. Each row is an estimated state at the corresponding time in `tSpan`. The simplest usage is then `x = PIRK4(microBurst,tSpan,x0,bT)`.

However, microscale details of the underlying Projective Integration computations may be helpful. `PIRK4()` provides up to four optional outputs of the microscale bursts.

- `tms`, optional, is an L dimensional column vector containing the microscale times within the burst simulations, each burst separated by `NaN`;
- `xms`, optional, is an $L \times n$ array of the corresponding microscale states—each rows is an accurate estimate of the state at the corresponding time `tms` and helps visualise details of the solution.
- `rm`, optional, a struct containing the ‘remaining’ applications of the `microBurst` required by the Projective Integration method during the calculation of the macrostep:
 - `rm.t` is a column vector of microscale times; and
 - `rm.x` is the array of corresponding burst states.

The states `rm.x` do not have the same physical interpretation as those in `xms`; the `rm.x` are required in order to estimate the slow vector field during the calculation of the Runge–Kutta increments, and do *not* accurately approximate the macroscale dynamics.

- `svf`, optional, a struct containing the Projective Integration estimates of the slow vector field.
 - `svf.t` is a 4ℓ dimensional column vector containing all times at which the Projective Integration scheme is extrapolated along `microBurst` data to form a macrostep.
 - `svf.dx` is a $4\ell \times n$ array containing the estimated slow vector field.

2.5.2 The projective integration code

Determine the number of time-steps and preallocate storage for macroscale estimates.

```
194 nT = length(tSpan);
195 x = nan(nT,length(x0));
```

Get the number of expected outputs and set logical indices to flag what data should be saved.

```
203 nArgOut = nargin();
204 saveMicro = (nArgOut>1);
205 saveFullMicro = (nArgOut>3);
206 saveSvf = (nArgOut>4);
```

Run a preliminary application of the micro-burst on the initial state to help relax to the slow manifold. This is done in addition to the micro-burst in the main loop, because the initial state is often far from the attracting slow manifold. Require the user to input and output rows of the system state.

```
219 x0 = reshape(x0,1,[]);
220 [relax_t,relax_x0] = microBurst(tSpan(1),x0,bT);
```

Use the end point of the micro-burst as the initial state for the macroscale time-steps.

```
228 tSpan(1) = relax_t(end);
229 x(1,:) = relax_x0(end,:);
```

If saving information, then record the first application of the micro-burst. Allocate cell arrays for times and states for outputs requested by the user, as concatenating cells is much faster than iteratively extending arrays.

```
239 if saveMicro
240     tms = cell(nT,1);
241     xms = cell(nT,1);
242     tms{1} = reshape(relax_t,[],1);
243     xms{1} = relax_x0;
244     if saveFullMicro
245         rm.t = cell(nT,1);
246         rm.x = cell(nT,1);
247         if saveSvf
248             svf.t = nan(4*nT-4,1);
249             svf.dx = nan(4*nT-4,length(x0));
250         end
251     end
252 end
```

Loop over the macroscale time-steps

```
260 for jT = 2:nT
261     T = tSpan(jT-1);
```

If four applications of the micro-burst would cover the entire macroscale time-step, then do so (setting some internal states to NaN); else proceed to projective step.

```
270 if ~isempty(bT) && 4*abs(bT)>=abs(tSpan(jT)-T) && bT*(tSpan(jT)-T)>0
271     [t1,xm1] = microBurst(T, x(jT-1,:), tSpan(jT)-T);
272     x(jT,:) = xm1(end,:);
```

```

273         t2=nan; xm2=nan(1,size(xm1,2));
274         t3=nan; t4=nan; xm3=xm2; xm4 = xm2; dx1=xm2; dx2=xm2;
275     else

```

Run the first application of the micro-burst; since this application directly follows from the initial conditions, or from the latest macrostep, this microscale information is physically meaningful as a simulation of the system. Extract the size of the final time-step.

```

286     [t1,xm1] = microBurst(T, x(jT-1,:), bT);
287     del = t1(end)-t1(end-1);

```

Check for round-off error.

```

293     xt = [reshape(t1(end-1:end),[],1) xm1(end-1:end,:)];
294     roundingTol = 1e-8;
295     if norm(diff(xt))/norm(xt,'fro') < roundingTol
296     warning(['significant round-off error in 1st projection at T=' num2str(T)
297     end

```

Find the needed time-step to reach time $tSpan(n+1)$ and form a first estimate $dx1$ of the slow vector field.

```

306     Dt = tSpan(jT)-t1(end);
307     dx1 = (xm1(end,:)-xm1(end-1,:))/del;

```

Assume burst times are the same length for this macro-step, or effectively so (recall that bT may be empty as it may be only coded and known in `microBurst()`).

```
316     abT = t1(end)-t1(1);
```

Project along $dx1$ to form an intermediate approximation of x ; run another application of the micro-burst and form a second estimate of the slow vector field.

```

327     xint = xm1(end,:)+(Dt/2-abT)*dx1;
328     [t2,xm2] = microBurst(T+Dt/2, xint, bT);
329     del = t2(end)-t2(end-1);
330     dx2 = (xm2(end,:)-xm2(end-1,:))/del;
331
332     xint = xm1(end,:)+(Dt/2-abT)*dx2;
333     [t3,xm3] = microBurst(T+Dt/2, xint, bT);
334     del = t3(end)-t3(end-1);
335     dx3 = (xm3(end,:)-xm3(end-1,:))/del;
336
337     xint = xm1(end,:)+(Dt-abT)*dx3;
338     [t4,xm4] = microBurst(T+Dt, xint, bT);
339     del = t4(end)-t4(end-1);
340     dx4 = (xm4(end,:)-xm4(end-1,:))/del;

```

Check for round-off error.

```

346     xt = [reshape(t2(end-1:end),[],1) xm2(end-1:end,:)];
347     if norm(diff(xt))/norm(xt,'fro') < roundingTol

```

```

348     warning(['significant round-off error in 2nd projection at T=' num2str(T))
349     end

```

Use the weighted average of the estimates of the slow vector field to take a macrostep.

```

357     x(jT,:) = xm1(end,:)+Dt*(dx1+2*dx2+2*dx3+dx4)/6;

```

Now end the if-statement that tests whether a projective step saves simulation time.

```

365     end

```

If saving trusted microscale data, then populate the cell arrays for the current loop iterate with the time-steps and output of the first application of the micro-burst. Separate bursts by NaNs.

```

375     if saveMicro
376         tms{jT} = [reshape(t1,[],1); nan];
377         xms{jT} = [xm1; nan(1,size(xm1,2))];

```

If saving all microscale data, then repeat for the remaining applications of the micro-burst.

```

385     if saveFullMicro
386         rm.t{jT} = [reshape(t2,[],1); nan;...
387                     reshape(t3,[],1); nan;...
388                     reshape(t4,[],1); nan];
389         rm.x{jT} = [xm2; nan(1,size(xm2,2));...
390                     xm3; nan(1,size(xm2,2));...
391                     xm4; nan(1,size(xm2,2))];

```

If saving Projective Integration estimates of the slow vector field, then populate the corresponding cells with times and estimates.

```

400     if saveSvf
401         svf.t(4*jT-7:4*jT-4) = [t1(end); t2(end); t3(end); t4(end)];
402         svf.dx(4*jT-7:4*jT-4,:) = [dx1; dx2; dx3; dx4];
403     end
404     end
405 end

```

End of the main loop of all macro-steps.

```

411 end

```

Overwrite $x(1,:)$ with the specified initial state $tSpan(1)$.

```

420 x(1,:) = reshape(x0,1,[]);

```

For additional requested output, concatenate all the cells of time and state data into two arrays.

```

428 if saveMicro
429     tms = cell2mat(tms);
430     xms = cell2mat(xms);
431     if saveFullMicro

```

```
432         rm.t = cell2mat(rm.t);  
433         rm.x = cell2mat(rm.x);  
434     end  
435 end
```

2.5.3 If no output specified, then plot the simulation

```
443 if nArgOut==0  
444     figure, plot(tSpan,x,'o:')
```

title('Projective Simulation with PIRK4')

```
445 end  
446  
453 end
```

This concludes PIRK4().

2.6 `cdmc()`: constraint defined manifold computing

The function `cdmc()` iteratively applies the given micro-burst and then projects backward to the initial time. The cumulative effect is to relax the variables to the attracting slow manifold, while keeping the ‘final’ time for the output the same as the input time.

```
17 function [ts, xs] = cdmc(microBurst, t0, x0)
```

Input

- `microBurst()`, a black-box micro-burst function suitable for Projective Integration. See any of `PIRK2()`, `PIRK4()`, or `PIG()` for a description of `microBurst()`.
- `t0`, an initial time.
- `x0`, an initial state vector.

Output

- `ts`, a vector of times.
- `xs`, an array of state estimates produced by `microBurst()`.

This function is a wrapper for the micro-burst. For instance if the problem of interest is a dynamical system that is not too stiff, and which is simulated by the micro-burst function `sol(t,x)`, one would invoke `cdmc()` by defining

```
cdmcSol = @(t,x) cdmc(sol,t,x)|
```

and thereafter use `cdmcSol()` in place of `sol()` as the microBurst in any Projective Integration scheme. The original microBurst `sol()` could create large errors if used in the `PIG()` scheme, but the output via `cdmc()` should not.

Begin with a standard application of the micro-burst. Need `feval` as `microBurst` has multiple outputs.

```
56 [t1,x1] = feval(microBurst,t0,x0);
57 bT = t1(end)-t1(1);
```

Project backwards to before the initial time, then simulate just one burst forward to obtain a simulation burst that ends at the original `t0`.

```
66 dxdt = (x1(end,:) - x1(end-1,:))/(t1(end) - t1(end-1));
67 x0 = x1(end,:)-2*bT*dxdt;
68 t0 = t1(1)-bT;
69 [t2,x2] = feval(microBurst,t0,x0.');
```

Return both sets of output(?), although only `(t2,x2)` should be used in Projective Integration—maybe safer to return only `(t2,x2)`.

```
77 ts = [t1(:); t2(:)];
78 xs = [x1; x2];
```

2.7 Example: PI using Runge–Kutta macrosolvers

This script demonstrates the PIRK4() scheme that uses a Runge–Kutta macrosolver, applied to simple linear systems with some slow and fast directions.

Clear workspace and set a seed.

```
15 clear
16 rand('seed',1) % albeit discouraged in Matlab
17 global dxdt
```

The majority of this example involves setting up details for the microsolver. We use a simple function gen_linear_system() that outputs a function $f(t, x) = A\vec{x} + \vec{b}$, where matrix A has some eigenvalues with large negative real part, corresponding to fast variables, and some eigenvalues with real part close to zero, corresponding to slow variables. The function gen_linear_system() requires that we specify bounds on the real part of the strongly stable eigenvalues,

```
32 fastband = [-5e2; -1e2];
```

and bounds on the real part of the weakly stable/unstable eigenvalues,

```
39 slowband = [-0.002; 0.002];
```

We now generate a random linear system with seven fast and three slow variables.

```
46 dxdt = gen_linear_system(7,3,fastband,slowband);
```

Set the macroscale times at which we request output from the PI scheme and the initial state.

```
56 tSpan = 0:1:20;
57 x0 = linspace(-10,10,10)';
```

We implement the PI scheme, saving the coarse states in \mathbf{x} , the ‘trusted’ applications of the microsolver in \mathbf{tms} and \mathbf{xms} , and the additional applications of the microsolver in \mathbf{rm} (the second, third and fourth outputs are optional).

```
70 [x, tms, xms, rm] = PIRK4(@linearBurst, tSpan, x0);
```

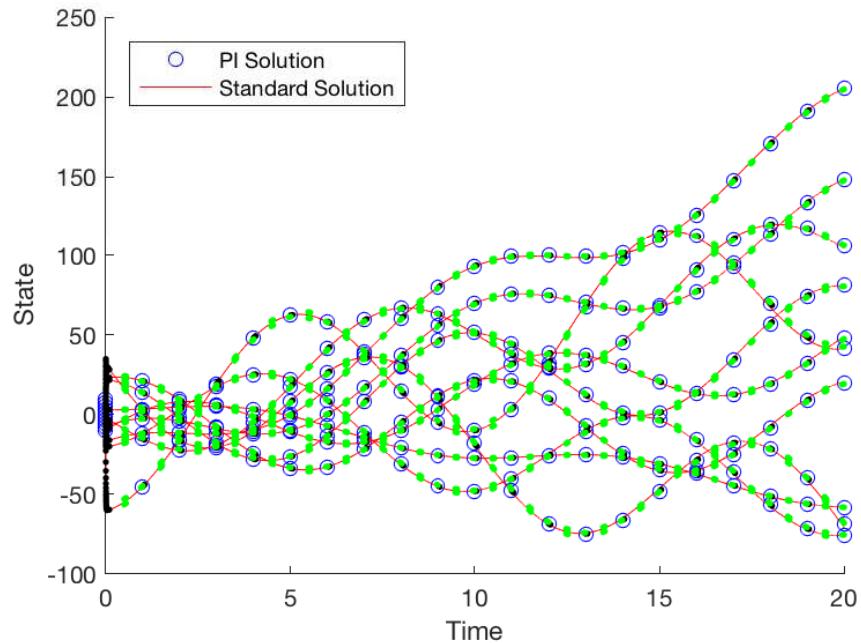
To verify, we also compute the trajectories using a standard integrator.

```
77 if ~exist('OCTAVE_VERSION','builtin')
78     [tt,xode] = ode45(dxdt,tSpan([1,end]),x0);
79 else % octave version
80     tt = linspace(tSpan(1),tSpan(end),101);
81     xode = lsode(@(x,t) dxdt(t,x),x0,tt);
82 end
```

[Figure 2.8](#) plots the output.

```
98 clf()
99 hold on
100 PI_sol=plot(tSpan,x,'bo');
101 std_sol=plot(tt,xode,'r');
```

Figure 2.8: Demonstration of PIRK4(). From initial conditions, the system rapidly transitions to an attracting invariant manifold. The PI solution accurately tracks the evolution of the variables over time while requiring only a fraction of the computations of the standard solver.



```

102 plot(tms,xms,'k.', rm.t,rm.x,'g.');
103 legend([PI_sol(1),std_sol(1)],'PI Solution',...
104     'Standard Solution','Location','NorthWest')
105 xlabel('Time'), ylabel('State')

Save plot to a file.

111 if ~exist('OCTAVE_VERSION','builtin')
112 set(gcf,'PaperUnits','centimeters','PaperPosition',[0 0 14 10])
113 print('-depsc2','PIRKexample')
114 end

```

A micro-burst simulation Used by `PIRKexample.m`. Code the micro-burst function using simple Euler steps. As a rule of thumb, the time-steps dt should satisfy $dt \leq 1/|\text{fastband}(1)|$ and the time to simulate with each application of the microsolver, bT , should be larger than or equal to $1/|\text{fastband}(2)|$. We set the integration scheme to be used in the microsolver. Since the time-steps are so small, we just use the forward Euler scheme

```

17 function [ts, xs] = linearBurst(ti, xi, varargin)
18 global dxdt
19 dt = 0.001;
20 ts = ti+(0:dt:0.05)';
21 nts = length(ts);
22 xs = NaN(nts,length(xi));

```

```
23 xs(1,:)=xi;
24 for k=2:nts
25     xi = xi + dt*dxdt(ts(k),xi.')';
26     xs(k,:)=xi;
27 end
28 end
```

2.8 Example: Projective Integration using General macrosolvers

In this example the Projective Integration-General scheme is applied to a singularly perturbed ordinary differential equation. The aim is to use a standard non-stiff numerical integrator, such as `ode45()`, on the slow, long-time macroscale. For this stiff system, `PIG()` is an order of magnitude faster than ordinary use of `ode45`.

```
18 clear all, close all
```

Set time scale separation and the underlying ODES:

$$\frac{dx_1}{dt} = \cos x_1 \sin x_2 \cos t, \quad \frac{dx_2}{dt} = \frac{1}{\epsilon}(-x_2 + \cos x_1).$$

```
30 epsilon = 1e-4;
31 dxdt=@(t,x) [ cos(x(1))*sin(x(2))*cos(t)
32 (cos(x(1))-x(2))/epsilon ];
```

Set the ‘black-box’ microsolver to be an integration using a standard solver, and set the standard time of simulation for the microsolver.

```
41 bT = epsilon*log(1/epsilon);
42 if ~exist('OCTAVE_VERSION','builtin')
43     micB='ode45'; else micB='rk2Int'; end
44 microBurst = @(tb0, xb0) feval(micB,dxdt,[tb0 tb0+bT],xb0);
```

Set initial conditions, and the time to be covered by the macrosolver.

```
52 x0 = [1 0.9];
53 tSpan = [0 5];
```

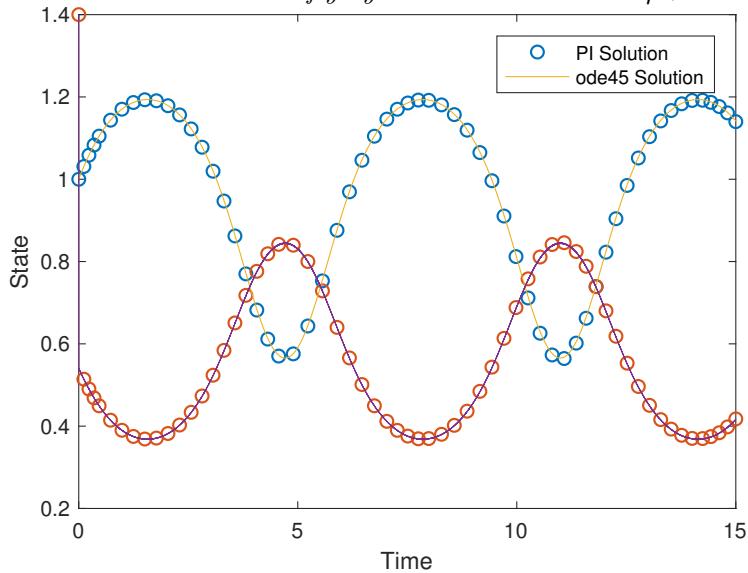
Now time and integrate the above system over `tSpan` using `PIG()` and, for comparison, a brute force implementation of `ode45/lsode`. Report the time taken by each method (in seconds).

```
62 if ~exist('OCTAVE_VERSION','builtin')
63     macInt='ode45'; else macInt='odeOct'; end
64 tic
65 [ts,xs,tms,xms] = PIG(macInt,microBurst,tSpan,x0);
66 secsPIGusingODEasMacro = toc
67 tic
68 [tClassic,xClassic] = feval(macInt,dxdt,tSpan,x0);
69 secsODEalone = toc
```

Plot the output on two figures, showing the truth and macrosteps on both, and all applications of the microsolver on the first figure.

```
79 figure
80 h = plot(ts,xs,'o', tClassic,xClassic,'-', tms,xms,'.');
81 legend(h(1:2:5),'Pro Int method','classic method','PI microsolver')
82 xlabel('Time'), ylabel('State')
83
84 figure
85 h = plot(ts,xs,'o', tClassic,xClassic,'-');
```

Figure 2.9: Accurate simulation of a stiff nonautonomous system by PIG(). The microsolver is called on-the-fly by the macrosolver `ode45/lode`.



```

86 legend(h([1 3]),'Pro Int method','classic method')
87 xlabel('Time'), ylabel('State')
88 if ~exist('OCTAVE_VERSION','builtin')
89 set(gcf,'PaperUnits','centimeters','PaperPosition',[0 0 14 10])
90 %print('-depsc2','PIGExample')
91 end

```

Figure 2.9 plots the output.

- The problem may be made more stiff or less stiff by changing the time-scale separation parameter $\epsilon = \text{epsilon}$. The compute time of `PIG()` is almost independent of ϵ , whereas that of `ode45()` is proportional to $1/\epsilon$.

If the problem is ‘semi-stiff’ (larger ϵ), then `PIG()`’s default of using `cdmc()` avoids nonsense ([Section 2.9](#)).

- The stiff but low dimensional problem in this example may be solved efficiently by a standard stiff solver (e.g., `ode15s()`). The real advantage of the Projective Integration schemes is in high dimensional stiff problems, that are not efficiently solved by most standard methods.

2.9 Explore: Projective Integration using constraint-defined manifold computing

In this example the Projective Integration-General scheme is applied to a singularly perturbed ordinary differential equation in which the time scale separation is not large. The results demonstrate the value of the default `cdmc()` wrapper for the microsolver.

```
16 clear all, close all
```

Set a weak time scale separation, and the underlying ODES:

$$\frac{dx_1}{dt} = \cos x_1 \sin x_2 \cos t, \quad \frac{dx_2}{dt} = \frac{1}{\epsilon}(-x_2 + \cos x_1).$$

```
28 epsilon = 0.01;
29 dxdt=@(t,x) [ cos(x(1))*sin(x(2))*cos(t)
30             (cos(x(1))-x(2))/epsilon ];
```

Set the microsolver to be an integration using a standard solver, and set the standard time of simulation for the microsolver.

```
39 bT = epsilon*log(1/epsilon);
40 if ~exist('OCTAVE_VERSION','builtin')
41     micB='ode45'; else micB='rk2Int'; end
42 microBurst = @(tb0, xb0) feval(micB,dxdt,[tb0 tb0+bT],xb0);
```

Set initial conditions, and the time to be covered by the macrosolver.

```
50 x0 = [1 0];
51 tSpan=0:0.5:15;
```

Simulate using `PIG()`, first without the default treatment of `cdmc` for the microsolver and second with. Generate a trusted solution using standard numerical methods.

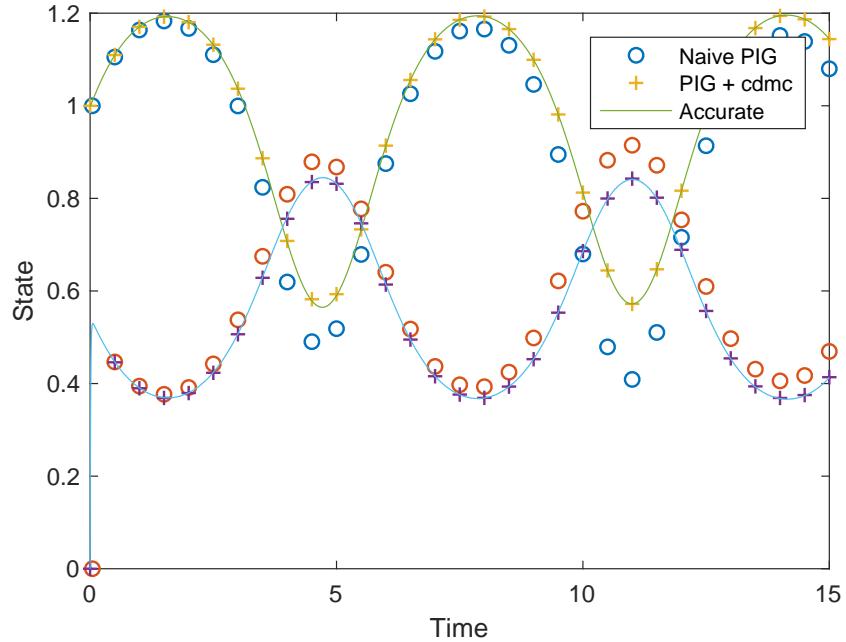
```
62 if ~exist('OCTAVE_VERSION','builtin')
63     macInt='ode45'; else macInt='odeOct'; end
64 [nt,nx] = PIG(macInt,microBurst,tSpan,x0,[],[],'no cdmc');
65 [ct,cx] = PIG(macInt,microBurst,tSpan,x0);
66 [tClassic,xClassic] = feval(macInt,dxdt,tSpan,x0);
```

[Figure 2.10](#) plots the output.

```
83 figure
84 h = plot(nt,nx,'rx', ct,cx,'bo', tClassic,xClassic,'-');
85 legend(h(1:2:5),'Naive PIG','PIG + cdmc','Accurate')
86 xlabel('Time'), ylabel('State')
87 if ~exist('OCTAVE_VERSION','builtin')
88 set(gcf,'PaperUnits','centimeters','PaperPosition',[0 0 14 10])
89 %print('-depsc2','PIGExplore')
90 end
```

A source of error in the standard `PIG()` scheme is the finite length of each burst, `bT`. This computes a time derivative at a time that is significantly different to that requested by standard coded schemes. Set `bT` to `20*epsilon`

Figure 2.10: Accurate simulation of a weakly stiff non-autonomous system by PIG() using cdm(), and an inaccurate solution using a naive application of PIG().



or `50*epsilon`¹ to worsen the error in both schemes. This example reflects a general principle: most Projective Integration schemes incur a global error term proportional to the burst time of the microsolver and independent of the order of the microsolver. The PIRK_n() schemes are written to eliminate this error, but PIG() works with any user-defined macrosolver and cannot reduce this error, except by using the function `cdm()`, its default.

¹ This example is quite extreme: at `bT=50*epsilon`, it would be computationally much cheaper to simulate the entire length of `tSpan` using the microsolver alone.

2.10 To do/discuss

- Implement lifting and restriction for PIRK_n() functions.
- Could implement Projective Integration by ‘arbitrary’ Runge–Kutta scheme; that is, by having the user input a particular Butcher table—surely only specialists would be interested.
- Can maybe implement microsolvers that terminate a burst when the fast dynamics have settled using, for example, the ‘Events’ function handle in ode23.
- Need projective integration of systems with fast oscillations, perhaps by DMD.
- Need projective integration for stochastic systems.

3 Patch scheme for given microscale discrete space system

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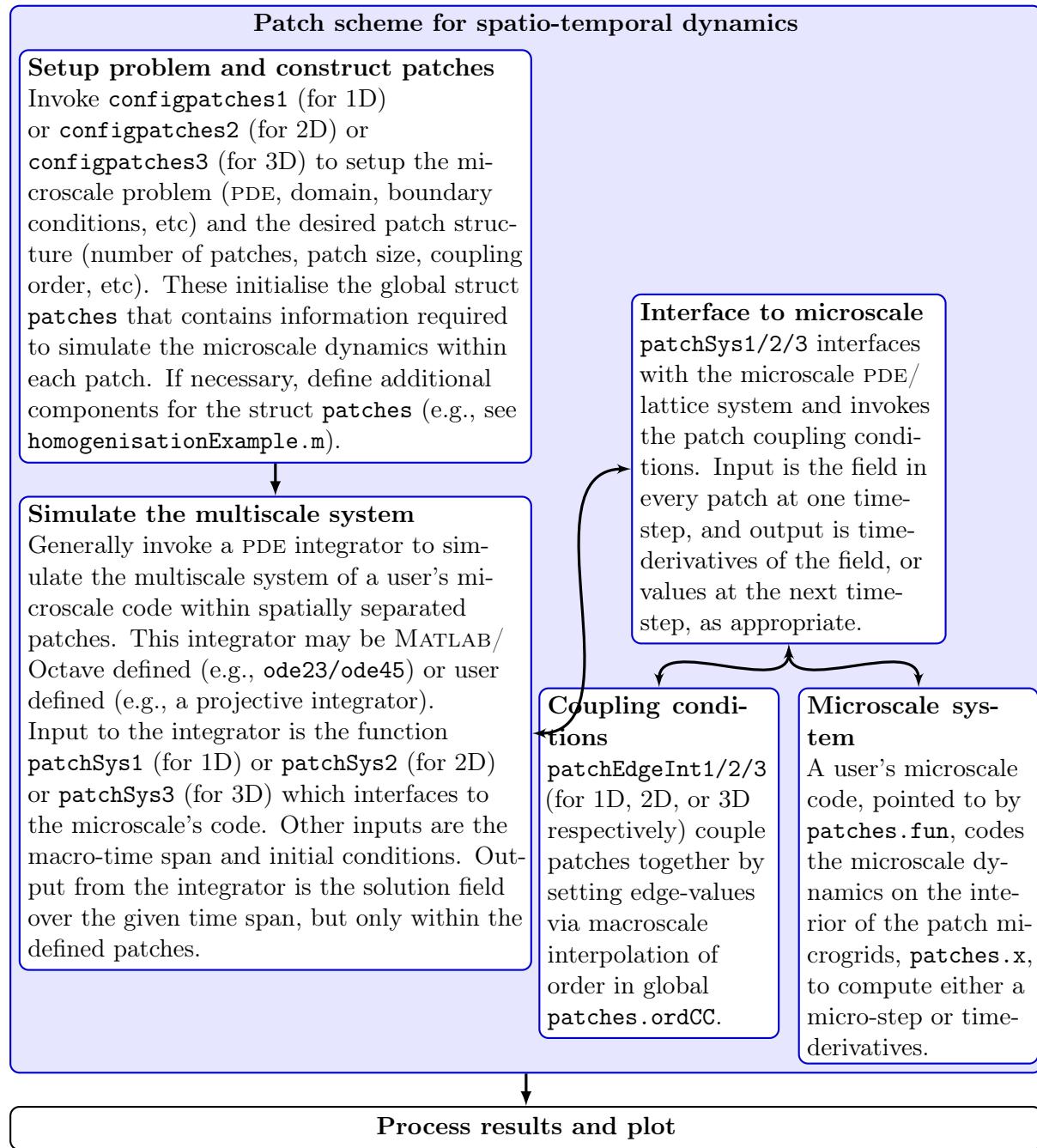
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Consider spatio-temporal multiscale systems where the spatial domain is so large that a given microscale code cannot be computed in a reasonable time. The *patch scheme* computes the microscale details only on small patches of the space-time domain, and produce correct macroscale predictions by craftily coupling the patches across unsimulated space (Hyman 2005, Samaey et al. 2005, 2006, Roberts & Kevrekidis 2007, Liu et al. 2015, e.g.). The resulting macroscale predictions were generally proved to be consistent with the microscale dynamics, to some specified order of accuracy, in a series of papers: 1D-space dissipative systems (Roberts & Kevrekidis 2007, Bunder et al. 2017); 2D-space dissipative systems (Roberts et al. 2014, Bunder et al. 2020); and 1D-space wave-like systems (Cao & Roberts 2016b).

The microscale spatial structure is to be on a lattice such as obtained from finite difference/element/volume approximation of a PDE. The microscale is either continuous or discrete in time.

Quick start See Sections 3.1.1 and 4.1.1 which respectively list example basic code that uses the provided functions to simulate the 1D Burgers' PDE, and a 2D nonlinear ‘diffusion’ PDE. Then see Figure 3.1.

Figure 3.1: The Patch methods, Chapter 3, accelerate simulation/integration of multiscale systems with interesting spatial/network structure/patterns. The methods use your given microsimulators whether coded from PDEs, lattice systems, or agent/particle microscale simulators. The patch functions require that a user configure the patches, and interface the coupled patches with a time integrator/simulator. This chart overviews the main functional recursion involved.



3.1 configPatches1(): configure spatial patches in 1D

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Makes the struct `patches` for use by the patch/gap-tooth time derivative/step function `patchSys1()`. [Section 3.1.1](#) lists an example of its use.

```
19 function patches = configPatches1(fun,Xlim,Dom ...
20     ,nPatch,ordCC,dx,nSubP,varargin)
21 version = '2023-03-23';
```

Input If invoked with no input arguments, then executes an example of simulating Burgers' PDE—see [Section 3.1.1](#) for the example code.

- `fun` is the name of the user function, `fun(t,u,patches)` or `fun(t,u)` or `fun(t,u,patches,...)`, 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 if 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—adjusted a little when `nEdge` > 1 . 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 `nSubP/nEdge` must be odd integer so that there is/are centre-patch lattice point(s). So for the defaults of `nEdge` = 1 and not `EdgyInt`, then `nSubP` must be odd.
- ‘`nEdge`’, *optional*, default=1, 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. Best accuracy usually obtained when the periodicity of the coefficients is a factor of `nSubP-2*nEdge` for `EdgyInt`, or a factor of $(nSubP-nEdge)/2$ for not `EdgyInt`.
 - 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.¹

```
187 if nargout==0, global patches, end
188 patches.version = version;
```

- `.fun` is the name of the user's function `fun(t,u,patches)` or `fun(t,u)` or `fun(t,u,patches,...)`, 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`.
- `.x` (4D) is `nSubP` \times 1 \times 1 \times `nPatch` array of the regular spatial locations x_{iI} of the i th microscale grid point in the I th patch.
- `.ratio`, only for macro-periodic conditions, is the size ratio of every patch.

¹ When using `spmd` parallel computing, it is generally best to avoid global variables, and so instead prefer using an explicit output variable.

- `.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.

3.1.1 If no arguments, then execute an example

```
261 if nargin==0
262 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.

```
282 global patches
283 patches = configPatches1(@BurgersPDE, [0 2*pi], ...
284     'periodic', 8, 0, 0.06, 7);
```

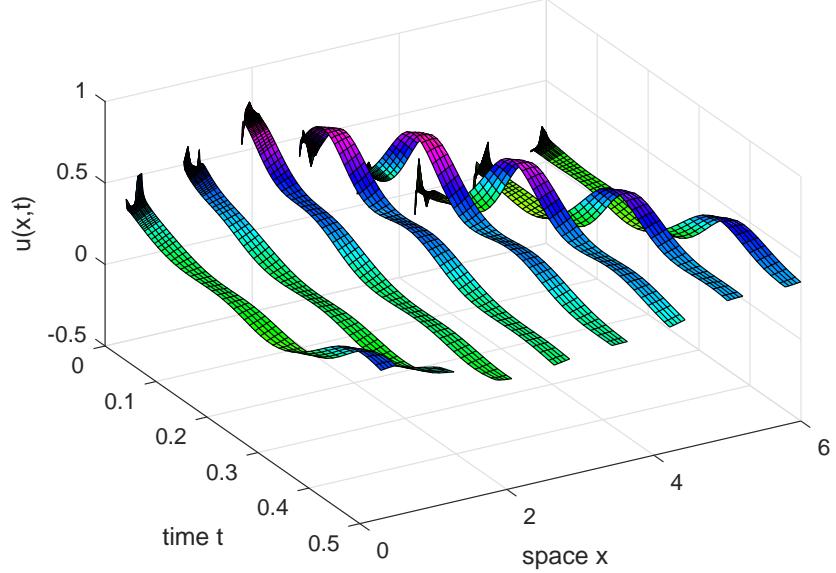
Set some initial condition, with some microscale randomness.

```
290 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()` ([Section 3.2](#)).

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

*Figure 3.2: field $u(x, t)$ of the patch scheme applied to Burgers' PDE.
Burgers PDE: patches in space, continuous time*



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 3.2](#) illustrates an example simulation in time generated by the patch scheme applied to Burgers' PDE.

```

314 figure(1),clf
315 if 1, patches.x([1 end],:,:, :)=nan; us=us.';
316 else us=reshape(patchEdgyInt1(us.'),[],length(ts));
317 end
318 mesh(ts,patches.x(:,us)
319 view(60,40), colormap(0.7*hsv)
320 title('Burgers PDE: patches in space, continuous time')
321 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 3.2](#), then exit this function.

```

335 ifOurCf2eps(mfilename)
336 return
337 end%if nargin==0

```

Example of Burgers PDE inside patches As a microscale discretisation of Burgers' PDE $u_t = u_{xx} - 30uu_x$, here code $\dot{u}_{ij} = \frac{1}{\delta x^2}(u_{i+1,j} - 2u_{i,j} + u_{i-1,j}) - 30u_{ij}\frac{1}{2\delta x}(u_{i+1,j} - u_{i-1,j})$. Here there is only one field variable, and one in the ensemble, so for simpler coding of the PDE we squeeze them out (with no need to reshape when via `patchSys1()`).

```

15 function ut=BurgersPDE(t,u,patches)
16     u=squeeze(u);      % omit singleton dimensions
17     dx=diff(patches.x(1:2)); % microscale spacing

```

```

18     i=2:size(u,1)-1; % interior points in patches
19     ut=nan+u;          % preallocate output array
20     ut(i,:)=diff(u,2)/dx^2 ...
21         -30*u(i,:).* (u(i+1,:)-u(i-1,:))/(2*dx);
22 end

10    function [ts,xs] = odeOcts(dxdt,tSpan,x0)
11        if length(tSpan)>2, ts = tSpan;
12        else ts = linspace(tSpan(1),tSpan(end),21)';
13        end
14        lsode_options('integration method','non-stiff');
15        xs = lsode(@(x,t) dxdt(t,x),x0,ts);
16    end

```

3.1.2 Parse input arguments and defaults

```

352 p = inputParser;
353 fnValidation = @(f) isa(f, 'function_handle'); %test for fn name
354 addRequired(p,'fun',fnValidation);
355 addRequired(p,'Xlim',@isnumeric);
356 %addRequired(p,'Dom'); % nothing yet decided
357 addRequired(p,'nPatch',@isnumeric);
358 addRequired(p,'ordCC',@isnumeric);
359 addRequired(p,'dx',@isnumeric);
360 addRequired(p,'nSubP',@isnumeric);
361 addParameter(p,'nEdge',1,@isnumeric);
362 addParameter(p,'EdgyInt',false,@islogical);
363 addParameter(p,'nEnsem',1,@isnumeric);
364 addParameter(p,'hetCoeffs',[],@isnumeric);
365 addParameter(p,'parallel',false,@islogical);
366 addParameter(p,'nCore',1,@isnumeric);
367 parse(p,fun,Xlim,nPatch,ordCC,dx,nSubP,varargin{:});

```

Set the optional parameters.

```

373 patches.nEdge = p.Results.nEdge;
374 patches.EdgyInt = p.Results.EdgyInt;
375 patches.nEnsem = p.Results.nEnsem;
376 cs = p.Results.hetCoeffs;
377 patches.parallel = p.Results.parallel;
378 patches.nCore = p.Results.nCore;

```

Check parameters.

```

385 assert(Xlim(1)<Xlim(2) ...
386     , 'two entries of Xlim must be ordered increasing')
387 assert((mod(ordCC,2)==0)|(patches.nEdge==1) ...
388     , 'Cannot yet have nEdge>1 and staggered patch grids')
389 assert(3*patches.nEdge<=nSubP ...
390     , 'too many edge values requested')
391 assert(rem(nSubP,patches.nEdge)==0 ...

```

```

392      , 'nSubP must be integer multiple of nEdge')
393  if ~patches.EdgyInt, assert(rem(nSubP/patches.nEdge,2)==1 ...
394      , 'for non-edgyInt, nSubP/nEdge must be odd integer')
395  end
396  if (patches.nEnsem>1)&(patches.nEdge>1)
397      warning('not yet tested when both nEnsem and nEdge non-one')
398  end
399  if patches.nCore>1
400      warning('nCore>1 not yet tested in this version')
401  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.

```

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

```

Default macroscale conditions are periodic with evenly spaced patches.

```

421  if isempty(Dom), Dom=struct('type','periodic'); end
422  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.

```

430  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.

```

438  patches.periodic=false;
439  switch Dom.type
440  case 'periodic'
441      patches.periodic=true;
442      if isfield(Dom,'bcOffset')
443          warning('bcOffset not available for Dom.type = periodic'), end
444      if isfield(Dom,'X')
445          warning('X not available for Dom.type = periodic'), end
446  case {'equispace','chebyshev'}
447      if ~isfield(Dom,'bcOffset'), Dom.bcOffset=[0;0]; end
448      if length(Dom.bcOffset)==1
449          Dom.bcOffset=repmat(Dom.bcOffset,2,1); end
450      if isfield(Dom,'X')
451          warning('X not available for Dom.type = equispace or chebyshev')
452      end
453  case 'usergiven'
454      if isfield(Dom,'bcOffset')
455          warning('bcOffset not available for usergiven Dom.type'), end
456          assert(isfield(Dom,'X'), 'X required for Dom.type = usergiven')
457  otherwise
458      error(['Dom.type ', ' is unknown Dom.type'])
459  end%switch Dom.type

```

3.1.3 The code to make patches and interpolation

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

```
471 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 .

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

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

```
488 patches.stag=mod(ordCC,2);
489 ordCC=ordCC+patches.stag;
490 patches.ordCC=ordCC;
```

Check for staggered grid and periodic case.

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

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

```
507 switch Dom.type
```

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

```
515 case 'periodic'
516 X=linspace(Xlim(1),Xlim(2),nPatch+1);
517 DX=X(2)-X(1);
518 X=X(1:nPatch)+diff(X)/2;
519 pEI=patches.EdgyInt;% abbreviation
520 pnE=patches.nEdge; % abbreviation
521 if pre2023, dx = ratio*DX/(nSubP-pnE*(1+pEI))*(2-pEI);
522 else      ratio = dx/DX*(nSubP-pnE*(1+pEI))/(2-pEI); end
523 patches.ratio=ratio;
```

In the case of macro-periodicity, precompute the weightings to interpolate field values for coupling.²

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

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

² **ToDo:** Might sometime extend to coupling via derivative values.

```

544 case 'equispace'
545     X=linspace(Xlim(1)+((nSubP-1)/2-Dom.bcOffset(1))*dx ...
546                 ,Xlim(2)-((nSubP-1)/2-Dom.bcOffset(2))*dx ,nPatch);
547     DX=diff(X(1:2));
548     width=(1+patches.EdgyInt)/2*(nSubP-1-patches.EdgyInt)*dx;
549     if DX<width*0.999999
550         warning('too many equispace patches (double overlapping)')
551     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’.³

```

568 case 'chebyshev'
569     halfWidth=dx*(nSubP-1)/2;
570     X1 = Xlim(1)+halfWidth-Dom.bcOffset(1)*dx;
571     X2 = Xlim(2)-halfWidth+Dom.bcOffset(2)*dx;
572 % 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`. We need to find `b`, the number of patches ‘glued’ together at the boundaries.

```

581 pEI=patches.EdgyInt;% abbreviation
582 pnE=patches.nEdge; % abbreviation
583 width=(1+pEI)/2*(nSubP-pnE-pEI*pnE)*dx;
584 for b=0:2:nPatch-2
585     DXmin=(X2-X1-b*width)/2*( 1-cos(pi/(nPatch-b-1)) );
586     if DXmin>width, break, end
587 end%for
588 if DXmin<width*0.999999
589     warning('too many Chebyshev patches (mid-domain overlap)')
590 end

```

Assign the centre-patch coordinates.

```

596 X = [ X1+(0:b/2-1)*width ...
597             (X1+X2)/2-(X2-X1-b*width)/2*cos(linspace(0,pi,nPatch-b)) ...
598             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.

```

607 case 'usergiven'
608     X = reshape(Dom.X,1,[]);
609 end%switch Dom.type

```

³ 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??

Fourth, construct the microscale grid in each patch, centred about the given mid-points X . Reshape the grid to be 4D to suit dimensions (micro,Vars,Ens,macro).

```
619 xs = dx*( (1:nSubP)-mean(1:nSubP) );
620 patches.x = reshape( xs'+X ,nSubP,1,1,nPatch);
```

3.1.4 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 [Section 3.5](#)).

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

```
650 nE = patches.nEnsem;
651 patches.le = 1:nE;
652 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.

```
664 if ~isempty(cs)
665 [mx,nc] = size(cs);
666 nx = nSubP(1);
667 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.

```
675 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.

```
684 patches.nEnsem = mx;
685 patches.cs = nan(nx-1,nc,mx);
686 for i = 1:mx
687     is = (i:i+nx-2);
```

```

688         patches.cs(:,:,i) = cs(is,:);
689     end
690     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.

```

700     patches.le = mod((0:mx-1)' + mod(nx-2,mx),mx)+1;
701     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??

```

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

```

End the two if-statements.

```

718 end%if-else nEnsem>1
719 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*.⁴

```

738 if patches.parallel
739 % theparpool=gcp()
740 spmd

```

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

```

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

```

`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.

```

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

```

⁴ If subsequently outside `spmd`, then one must use functions like `getfield(patches{1}, 'a')`.

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

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

Fin

```
782 end% function
```

3.2 patchSys1(): interface 1D space to time integrators

To simulate in time with 1D spatial patches we often need to interface a user's time derivative function with time integration routines such as `ode23` or `PIRK2`. This function provides an interface. Communicate patch-design variables (Section 3.1) either via the global struct `patches` or via an optional third argument. `patches` is required for the parallel computing of `spmd`, or if parameters are to be passed though to the user microscale function.

```
23 function dudt=patchSys1(t,u,patches,varargin)
24 if nargin<3, global patches, end
```

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 $nSubP \times nPatch$ grid.
- `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,patches,...)` that computes the time derivatives on the patchy lattice. The array `u` has size `nSubP × nVars × nEnsem × 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 the microscale.
- `varargin`, optional, is arbitrary number of parameters to be passed onto the users time-derivative function as specified in `configPatches1`.

Output

- `dudt` is a vector/array of of time derivatives, but with patch edge-values set to zero. It is of total length `nSubP · nVars · nEnsem · nPatch` and the same dimensions as `u`.

Reshape the fields `u` as a 4D-array, and sets the edge values from macroscale interpolation of centre-patch values. Section 3.3 describes `patchEdgeInt1()`.

```
82 sizeu = size(u);
83 u = patchEdgeInt1(u,patches);
```

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.

```
93 dudt=patches.fun(t,u,patches,varargin{:});
94 n=patches.nEdge;
```

```
95 dudt([1:n end-n+1:end],:,:,:)=0;  
96 dudt=reshape(dudt,sizeu);
```

Fin.

3.3 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 & Kevrekidis 2007), or the patch-core average (Bunder et al. 2017), or the opposite next-to-edge values (Bunder et al. 2020)—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 et al. 2017).⁵

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
```

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 $nSubP \times 1 \times 1 \times nPatch$ 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).
 - `.nEdge`, for each patch, the number of edge values set by interpolation at the edge regions of each patch (default is one).

⁵ Script `patchEdgeInt1test.m` verifies this code.

- `.nEnsem` the number of realisations in the ensemble.
- `.parallel` whether serial or parallel.
- `.nCore`⁶

Output

- `u` is 4D array, $nSubP \times nVars \times nEnsem \times nPatch$, 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.

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

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

```
127 [nx,~,~,Nx] = size(patches.x);
128 nEnsem = patches.nEnsem;
129 nVars = round(numel(u)/numel(patches.x)/nEnsem);
130 assert(numel(u) == nx*nVars*nEnsem*Nx ...
131 , 'patchEdgeInt1: input u has wrong size for parameters')
132 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.

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

Implement multiple width edges by folding Subsample x coordinates, noting it is only differences that count *and* the microgrid x spacing must be uniform.

```
153 x = patches.x;
154 if patches.nEdge>1
155     nEdge = patches.nEdge;
156     x = x(1:nEdge:nx,:,:,:);
157     nx = nx/nEdge;
158     u = reshape(u,nEdge,nx,nVars,nEnsem,Nx);
159     nVars = nVars*nEdge;
160     u = reshape( permute(u,[2 1 3:5]) ,nx,nVars,nEnsem,Nx);
161 end%if patches.nEdge
```

⁶ **ToDo:** introduced sometime but not fully implemented yet, because prefer ensemble

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

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

3.3.1 Periodic macroscale interpolation schemes

```
180 if patches.periodic
```

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

```
187 r = patches.ratio(1);
188 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.

```
198 if patches.EdgeyInt % interpolate next-to-edge values
199     Ux = u([2 nx-1],:,:,I);
200 else % interpolate mid-patch values/sums
201     Ux = sum( u((i0-c):(i0+c),:,:,I) ,1);
202 end;
```

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

```
210 szUx0=size(Ux);
211 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.

```
220 if patches.parallel
221     dmu = zeros(szUx0,patches.codist); % 5D
222 else
223     dmu = zeros(szUx0); % 5D
224 end
```

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

```
231 if patches.stag % use only odd numbered neighbours
232     dmu(:,:,:,:,I,1) = (Ux(:,:,:,:,Ip)+Ux(:,:,:,:,Im))/2; % \mu
233     dmu(:,:,:,:,I,2) = (Ux(:,:,:,:,Ip)-Ux(:,:,:,:,Im)); % \delta
234     Ip = Ip(Ip); Im = Im(Im); % increase shifts to \pm2
235 else % standard
236     dmu(:,:,:,:,I,1) = (Ux(:,:,:,:,Ip)-Ux(:,:,:,:,Im))/2; % \mu\delta
237     dmu(:,:,:,:,I,2) = (Ux(:,:,:,:,Ip)-2*Ux(:,:,:,:,I) ...
238                           +Ux(:,:,:,:,Im)); % \delta^2
239 end%if patches.stag
```

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

```

246   for k = 3:patches.ordCC
247     dmu(:,:, :, :, k) =      dmu(:,:, :, Ip, k-2) ...
248       -2*dmu(:,:, I, k-2) + dmu(:,:, Im, k-2);
249   end

```

Interpolate macro-values to be Dirichlet edge values for each patch ([Roberts & Kevrekidis 2007](#), [Bunder et al. 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`.

```

264   if patches.nCore==1
265     k=1+patches.EdgyInt; % use centre/core or two edges
266     u(nx,:, patches.ri, I) = Ux(1,:,:,:)*(1-patches.stag) ...
267       +sum( shiftdim(patches.Cwtsr,-4).*dmu(1,:,:,:,:) ,5);
268     u(1,:, patches.le, I) = Ux(k,:,:,:)*(1-patches.stag) ...
269       +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.

```

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

```

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

```
297 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 N_x patches we resolve ‘wavenumbers’ $|k| < N_x/2$, so set row vector $\mathbf{ks} = k2\pi/N$ for ‘wavenumbers’ $k = (0, 1, \dots, k_{\max}, -k_{\max}, \dots, -1)$ for odd N , and $k = (0, 1, \dots, k_{\max}, (k_{\max}+1), -k_{\max}, \dots, -1)$ 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. ⁷ ⁸

```

323 if patches.stag % transform by doubling the number of fields
324   v = nan(size(u)); % currently to restore the shape of u
325   u = [u(:,:, :,1:2:Nx) u(:,:, :,2:2:Nx)];
326   stagShift = 0.5*[ones(1,nVars) -ones(1,nVars)];
327   iV = [nVars+1:2*nVars 1:nVars]; % scatter interp to alternate field
328   r = r/2; % ratio effectively halved
329   Nx = Nx/2; % halve the number of patches
330   nVars = nVars*2; % double the number of fields
331 else % the values for standard spectral
332   stagShift = 0;
333   iV = 1:nVars;
334 end%if patches.stag

```

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

```

341 kMax = floor((Nx-1)/2);
342 ks = shiftdim( ...
343   2*pi/Nx*(mod((0:Nx-1)+kMax,Nx)-kMax) ...
344   ,-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`.

```

357 if ~patches.EdgyInt
358   Cleft = fft(u(i0 ,:,:, :) ,[],4);
359   Cright = Cleft;
360 else
361   Cleft = fft(u(2 ,:,:, :) ,[],4);
362   Cright= fft(u(nx-1,:,:, :) ,[],4);
363 end

```

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

```

370 u(nx,iV,patches.ri,:) = uclean( ifft( ...
371   Cleft.*exp(1i*ks.*(stagShift+r)) ,[],4));
372 u(1 ,iV,patches.le,:) = uclean( ifft( ...
373   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?

```

381 if patches.stag
382   nVars = nVars/2;
383   u=reshape(u,nx,nVars,2,nEnsem,Nx);

```

⁷ **ToDo:** Have not yet tested whether works for Edgy Interpolation.

⁸ **ToDo:** Have not yet implemented multiple edge values for a staggered grid as I am uncertain whether it makes any sense.

```

384     Nx = 2*Nx;
385     v(:,:,1:2:Nx) = u(:,:,1,:,:);
386     v(:,:,2:2:Nx) = u(:,:,2,:,:);
387     u = v;
388 end%if patches.stag
389 end%if patches.ordCC

```

3.3.2 Non-periodic macroscale interpolation

```

397 else% patches.periodic false
398 assert(~patches.stag, ...
399 '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 .

```

406 if patches.ordCC<1, patches.ordCC = Nx-1; end
407 p = min(patches.ordCC,Nx-1);
408 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.

```

418 if patches.EdgyInt % interpolate next-to-edge values
419     F(:,:,:,1) = u([nx-1 2],:,:,I);
420     X(:,:,:, :) = x([nx-1 2],:,:,I);
421 else % interpolate mid-patch values/sums
422     F(:,:,:,1) = sum( u((i0-c):(i0+c),:,:,I) ,1);
423     X(:,:,:, :) = x(i0,:,:,:,I);
424 end;

```

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

```

432 for q = 1:p
433     i = 1:Nx-q;
434     F(:,:,:,i,q+1) = (F(:,:,:,i+1,q)-F(:,:,:,i,q)) ...
435         ./(X(:,:,:,i+q) -X(:,:,:,i));
436 end

```

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

```

442 Xedge = 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.⁹ First alternative: the case of order p interpolation across the domain, asymmetric near the boundary. Use this first alternative for now.

⁹ 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??

```

458 if true
459   i = max(1,min(1:Nx,Nx-ceil(p/2))-floor(p/2));
460   Uedge = F(:,:,i,p+1);
461   for q = p:-1:1
462     Uedge = F(:,:,i,q)+(Xedge-X(:,:,i+q-1)).*Uedge;
463   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. ¹⁰

```

474 else%if false
475   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.

```

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

```

Initialise to highest divide difference, surrounded by zeros.

```

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

```

Complete Horner evaluation of the relevant polynomials.

```

498 for q = p:-1:1
499   Q = [Q(2:Imid) true(1,2) Q(Imid+1:end-1)]; % spread mask
500   Uedge(:,:,:,:Q) = F(:,:,:,:i(Q),q) ...
501     +(Xedge(:,:,:,:Q)-X(:,:,:,:i(Q)+q-1)).*Uedge(:,:,:,:Q);
502 end%for q
503 end%if

```

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

```

511 u(1 ,:,patches.le,I) = Uedge(1,:,:,:I);
512 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, unless testing, override their computed interpolation values with NaN.

```

522 if isfield(patches,'intTest')&&patches.intTest
523 else % usual case
524   u( 1,:,:,: 1) = nan;
525   u(nx,:,:,:Nx) = nan;
526 end%if

```

End of the non-periodic interpolation code.

¹⁰ 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.

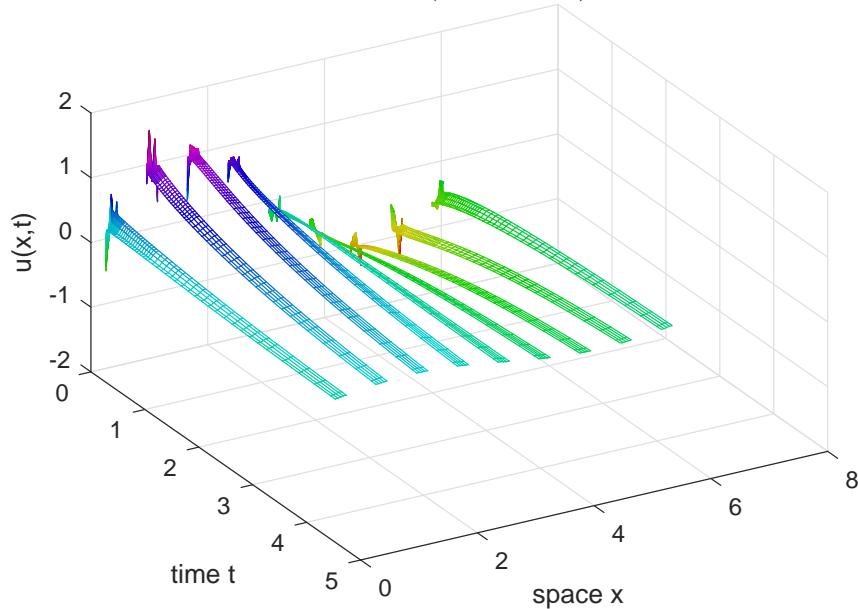
```
532 end%if patches.periodic
```

Unfold multiple edges No need to restore x .

```
539 if patches.nEdge>1
540   nVars = nVars/nEdge;
541   u = reshape( u ,nx,nEdge,nVars,nEnsem,Nx);
542   nx = nx*nEdge;
543   u = reshape( permute(u,[2 1 3:5]) ,nx,nVars,nEnsem,Nx);
544 end%if patches.nEdge
```

Fin, returning the 4D array of field values.

Figure 3.3: the diffusing field $u(x, t)$ in the patch (gap-tooth) scheme applied to microscale heterogeneous diffusion (Section 3.4).



3.4 homogenisationExample: simulate heterogeneous diffusion in 1D on patches

Section contents

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Figure 3.3 shows an example simulation in time generated by the patch scheme applied to heterogeneous diffusion. That such simulations of heterogeneous diffusion makes valid predictions was established by Bunder et al. (2017) who proved that the scheme is accurate when the number of points in a patch is one more than a multiple of the periodic of the microscale heterogeneity.

The first part of the script implements the following gap-tooth scheme (left-right arrows denote function recursion).

1. configPatches1
2. `ode15s` \mapsto patchSys1 \mapsto `heteroDiff`
3. process results

Consider a lattice of values $u_i(t)$, with lattice spacing dx , and governed by the heterogeneous diffusion

$$\dot{u}_i = [c_{i-1/2}(u_{i-1} - u_i) + c_{i+1/2}(u_{i+1} - u_i)]/dx^2. \quad (3.1)$$

In this 1D space, the macroscale, homogenised, effective diffusion should be the harmonic mean of these coefficients.

3.4.1 Script to simulate via stiff or projective integration

Set the desired microscale periodicity, and correspondingly choose random microscale diffusion coefficients (with subscripts shifted by a half).

```
53 mPeriod = 3
54 cDiff = exp(randn(mPeriod,1))
55 cHomo = 1/mean(1./cDiff)
```

Establish global data struct `patches` for heterogeneous diffusion on 2π -periodic domain. Use nine patches, each patch of half-size ratio 0.2. Quartic (fourth-order) interpolation `ordCC = 4` provides values for the inter-patch coupling conditions. Here include the diffusivity coefficients, repeated to fill up a patch.

```
67 global patches
68 nPatch = 9
69 ratio = 0.2
70 nSubP = 2*mPeriod+1
71 Len = 2*pi;
72 ordCC = 4;
73 configPatches1(@heteroDiff,[0 Len],nan,nPatch ...
74 ,ordCC,ratio,nSubP,'hetCoeffs',cDiff);
```

For comparison: conventional integration in time Set an initial condition, and here integrate forward in time using a standard method for stiff systems—because of the simplicity of linear problems this method works quite efficiently here. Integrate the interface `patchSys1` ([Section 3.2](#)) to the microscale differential equations.

```
88 u0 = sin(patches.x)+0.3*randn(nSubP,1,1,nPatch);
89 if ~exist('OCTAVE_VERSION','builtin')
90 [ts,ucts] = ode15s(@patchSys1, [0 2/cHomo], u0(:));
91 else % octave version
92 [ts,ucts] = odeOcts(@patchSys1, [0 2/cHomo], u0(:));
93 end
94 ucts = reshape(ucts,length(ts),length(patches.x(:)),[]);
```

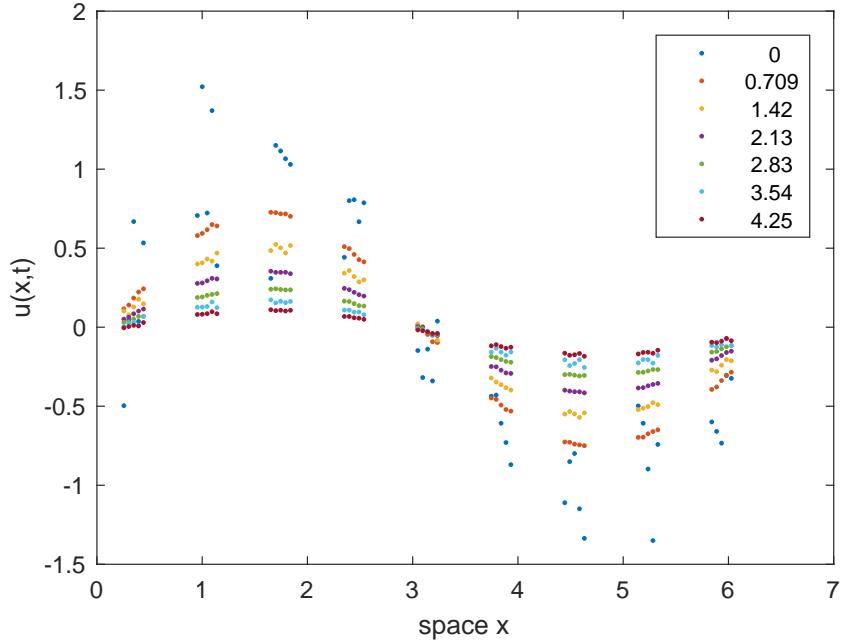
Plot the simulation in [Figure 3.3](#).

```
101 figure(1),clf
102 xs = patches.x; xs([1 end],:) = nan;
103 mesh(ts,xs(:,ucts')), view(60,40)
104 xlabel('time $t$'), ylabel('space $x$'), zlabel('$u(x,t)$')
105 ifOurCf2eps([mfilename 'CtsU'])
```

The code may invoke this integration interface.

```
10 function [ts,xs] = odeOcts(dxdt,tSpan,x0)
11     if length(tSpan)>2, ts = tSpan;
12     else ts = linspace(tSpan(1),tSpan(end),21)';
13     end
14     lsode_options('integration method','non-stiff');
```

Figure 3.4: field $u(x, t)$ shows basic projective integration of patches of heterogeneous diffusion: different colours correspond to the times in the legend. This field solution displays some fine scale heterogeneity due to the heterogeneous diffusion.



```

15      xs = lsode(@(x,t) dxdt(t,x),x0,ts);
16  end

```

Use projective integration in time Now take `patchSys1`, the interface to the time derivatives, and wrap around it the projective integration PIRK2 (Section 2.2), of bursts of simulation from `heteroBurst` (Section 3.4.3), as illustrated by Figure 3.4.

This second part of the script implements the following design, where the micro-integrator could be, for example, `ode45` or `rk2int`.

1. configPatches1 (done in first part)
2. PIRK2 \mapsto heteroBurst \mapsto micro-integrator \mapsto patchSys1 \mapsto heteroDiff
3. process results

Mark that edge of patches are not to be used in the projective extrapolation by setting initial values to NaN.

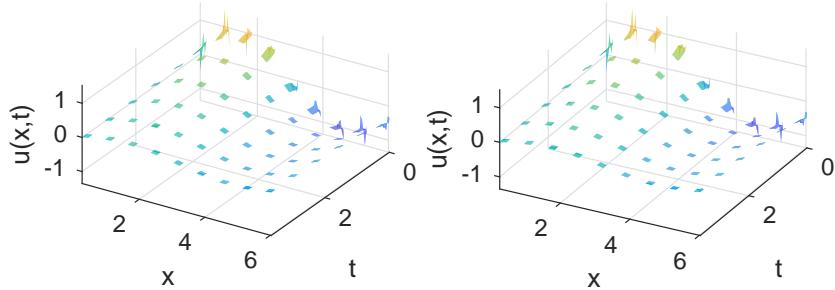
```

141 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; the burst time is proportional to the intra-patch effective diffusion time; and lastly, the microscale time-step is proportional to the diffusion time between adjacent points in the microscale lattice.

Figure 3.5: cross-eyed stereo pair of the field $u(x,t)$ during each of the microscale bursts used in the projective integration of heterogeneous diffusion.



```

153 ts = linspace(0,2/cHomo,7)
154 bT = 3*( ratio*Len/nPatch )^2/cHomo
155 addpath('..../ProjInt')
156 [us,tss,uss] = PIRK2(@heteroBurst, ts, u0(:), bT);

```

Plot the macroscale predictions to draw Figure 3.4.

```

163 figure(2),clf
164 plot(xs(:,us,'.')
165 ylabel('$u(x,t)$'), xlabel('space $x$')
166 legend(num2str(ts',3))
167 ifOurCf2eps([mfilename 'U'])

```

Also plot a surface detailing the microscale bursts as shown in the stereo Figure 3.5.

```

182 figure(3),clf
183 for k = 1:2, subplot(2,2,k)
184 surf(tss,xs(:,uss', 'EdgeColor','none')
185 ylabel('$x$'), xlabel('$t$'), zlabel('$u(x,t)$')
186 axis tight, view(126-4*k,45)
187 end
188 ifOurCf2eps([mfilename 'Micro'])

```

End of this example script.

3.4.2 heteroDiff(): heterogeneous diffusion

This function codes the lattice heterogeneous diffusion inside the patches. For 2D input arrays u and x (via edge-value interpolation of `patchSys1`, Section 3.2), computes the time derivative (3.1) at each point in the interior of a patch, output in ut . The column vector of diffusivities c_i , and possibly Burgers' advection coefficients b_i , have previously been stored in struct `patches.cs`.

```

21 function ut = heteroDiff(t,u,patches)
22 dx = diff(patches.x(2:3)); % space step
23 i = 2:size(u,1)-1; % interior points in a patch
24 ut = nan+u; % preallocate output array
25 ut(i,:,:,:) = diff(patches.cs(:,1,:).*diff(u))/dx.^2;

```

```

26    % possibly include heterogeneous Burgers' advection
27    if size(patches.cs,2)>1 % check for advection coeffs
28        buu = patches.cs(:,2,:).*u.^2;
29        ut(i,:) = ut(i,:)-(buu(i+1,:)-buu(i-1,:))/(dx*2);
30    end
31 end% function

```

3.4.3 heteroBurst(): a burst of heterogeneous diffusion

This code integrates in time the derivatives computed by `heteroDiff` from within the patch coupling of `patchSys1`. Try `ode23` or `rk2Int`, although `ode45` may give smoother results.

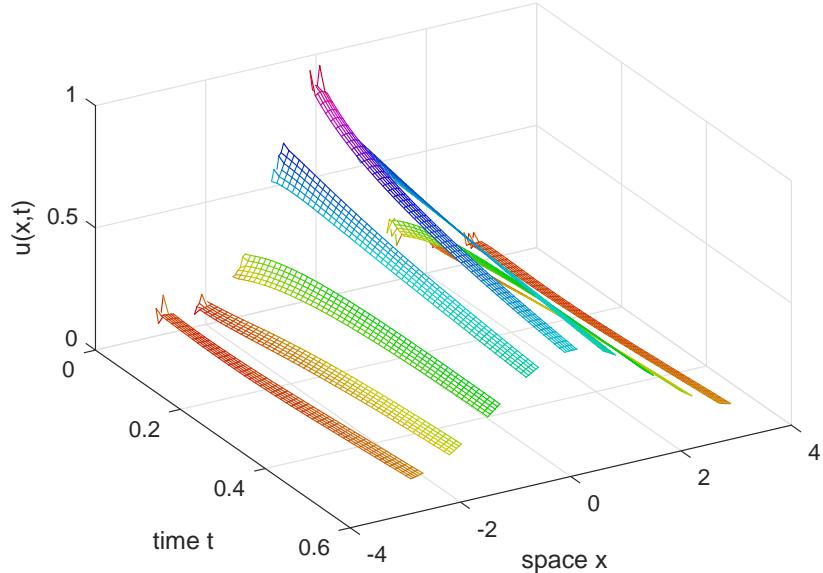
```

15 function [ts, ucts] = heteroBurst(ti, ui, bT)
16     if ~exist('OCTAVE_VERSION','builtin')
17         [ts,ucts] = ode23( @patchSys1,[ti ti+bT],ui(:));
18     else % octave version
19         [ts,ucts] = rk2Int(@patchSys1,[ti ti+bT],ui(:));
20     end
21 end

```

Fin.

Figure 3.6: diffusion field $u(x, t)$ of the gap-tooth scheme applied to the diffusion (3.2). The microscale random component to the initial condition, the sub-patch fluctuations, decays, leaving the emergent macroscale diffusion. This simulation uses nine patches of ‘large’ size ratio 0.25 for visibility.



3.5 homoDiffEdgy1: computational homogenisation of a 1D heterogeneous diffusion by simulation on small patches

Figure 3.6 shows an example simulation in time generated by the patch scheme applied to macroscale diffusion propagation through a medium with microscale heterogeneity. The inter-patch coupling is realised by quartic interpolation of the patch’s next-to-edge values to the patch opposite edges. Such coupling preserves symmetry in many systems, and quartic appears to be the lowest order that generally gives good accuracy.

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

$$\frac{\partial u_i}{\partial t} = \frac{1}{dx^2} \delta[c_{i+1/2} \delta u_i], \quad (3.2)$$

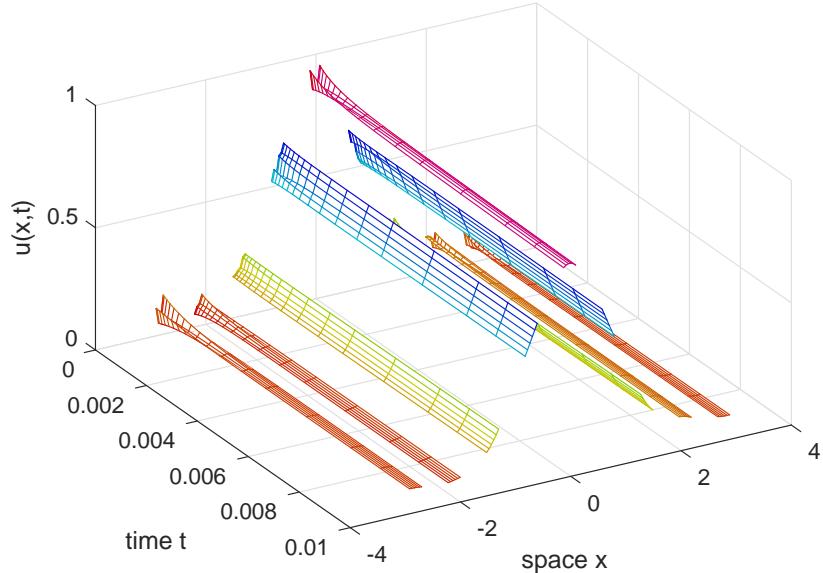
in terms of the centred difference operator δ . The system has a microscale heterogeneity via the coefficients $c_{i+1/2}$ which we assume to have some given known periodicity. Figure 3.6 shows one patch simulation of this system: observe the effects of the heterogeneity within each patch.

3.5.1 Script code to simulate heterogeneous diffusion systems

This example script implements the following patch/gap-tooth scheme (left-right arrows denote function recursion).

1. configPatches1
2. ode15s \mapsto patchSys1 \mapsto heteroDiff
3. plot the simulation

Figure 3.7: diffusion field $u(x,t)$ of the gap-tooth scheme applied to the diffusive (3.2). Over this short meso-time we see the macroscale diffusion emerging from the damped sub-patch fast quasi-equilibration.



4. use patchSys1 to explore the Jacobian

First establish the microscale heterogeneity has micro-period `mPeriod` on the lattice, and random log-normal values, albeit normalised to have harmonic mean one. This normalisation then means that macroscale diffusion on a domain of length 2π should have near integer decay rates, the squares of $0, 1, 2, \dots$. Then the heterogeneity is repeated to fill each patch, and phase-shifted for an ensemble.

```

90 mPeriod = 3%randi([2 5])
91 % set random diffusion coefficients
92 cHetr=exp(0.3*randn(mPeriod,1));
93 %cHetr = [3.966;2.531;0.838;0.331;7.276];
94 cHetr = cHetr*mean(1./cHetr) % normalise

```

Establish the global data struct `patches` for the microscale heterogeneous lattice diffusion system (3.2) solved on 2π -periodic domain, with seven patches, here each patch of size ratio 0.25 from one side to the other, with five micro-grid points in each patch, and quartic interpolation (4) to provide the edge-values of the inter-patch coupling conditions. Setting `patches.EdgeInt` to one means the edge-values come from interpolating the opposite next-to-edge values of the patches (not the mid-patch values). In this case we appear to need at least fourth order (quartic) interpolation to get reasonable decay rate for heterogeneous diffusion. When simulating an ensemble of configurations, `nSubP` (the number of points in a patch) need not be dependent on the period of the heterogeneous diffusion.

```

116 global patches
117 nPatch = 9
118 ratio = 0.25;

```

```

119 nSubP = mPeriod+1 %randi([mPeriod+1 2*mPeriod+2])
120 nEnsem = mPeriod % number realisations in ensemble
121 if mod(nSubP,mPeriod)==2, nEnsem=1, end
122 configPatches1(@heteroDiff, [-pi pi], nan, nPatch ...
123 , 4, ratio, nSubP, 'EdgyInt', true, 'nEnsem', nEnsem ...
124 , 'hetCoeffs', cHetr);

```

Simulate Set the initial conditions of a simulation to be that of a lump perturbed by significant random microscale noise, via `randn`.

```

135 u0 = 0.8*exp(-patches.x.^2)+0.2*rand(nSubP,1,nEnsem,nPatch);
136 du0dt = patchSys1(0,u0(:));

```

Integrate using standard integrators.

```

142 if ~exist('OCTAVE_VERSION','builtin')
143     [ts,us] = ode23(@patchSys1, [0 0.6], u0(:));
144 else % octave version
145     [ts,us] = odeOcts(@patchSys1, 0.6*linspace(0,1).^2, u0(:));
146 end

```

Plot space-time surface of the simulation We want to see the edge values of the patches, so we 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. In the case of an ensemble of phase-shifts, we plot the mean over the ensemble.

```

159 xs = squeeze(patches.x);
160 us = patchEdgeInt1( permute( reshape(us ...
161 ,length(ts),nSubP,nEnsem,nPatch) ,[2 1 3 4]) );
162 usstd = squeeze(std(us,0,3));
163 us = squeeze(mean(us,3));
164 if 0, % omit interpolated edges
165     us([1 end],:,:) = nan;
166     usstd([1 end],:,:) = nan;
167 else % insert nans between patches
168     xs(end+1,:)=nan;
169     us(end+1,:,:) = nan;
170     usstd(end+1,:,:) = nan;
171 end
172 us=reshape(permute(us,[1 3 2]),[],length(ts));
173 usstd=reshape(permute(usstd,[1 3 2]),[],length(ts));

```

Now plot two space-time graphs. The first is every time step over a meso-time to see the oscillation and decay of the fast sub-patch diffusions. The second is subsampled surface over the macroscale duration of the simulation to show the propagation of the macroscale diffusion over the heterogeneous lattice.

```

185 for p=1:2
186     switch p
187         case 1, j=find(ts<0.01);

```

```

188 case 2, [~,j]=min(abs(ts(:)-linspace(ts(1),ts(end),50)));
189 end
190 figure(p),clf
191 mesh(ts(j),xs(:,),us(:,j))
192 view(60,40), colormap(0.8*hsv)
193 xlabel('time $t$'), ylabel('space $x$'), zlabel('$u(x,t)$')
194 ifOurCf2eps([mfilename 'U' num2str(p)])
195 end
196 pause(3)

```

Compute Jacobian and its spectrum Let's explore the Jacobian dynamics for a range of orders of interpolation, all for the same patch design and heterogeneity. Here use a smaller ratio, and more patches, as we do not plot.

```

209 nPatch = 13
210 ratio = 0.01;
211
212 leadingEvals=[];
213 for ord=0:2:8
214     ordInterp=ord
215     configPatches1(@heteroDiff, [-pi pi], nan, nPatch ...
216         , ord, ratio, nSubP, 'EdgyInt', true, 'nEnsem', nEnsem ...
217         , 'hetCoeffs', cHetr);

```

Form the Jacobian matrix, 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.

```

227 u0 = zeros(nSubP,1,nEnsem,nPatch);
228 u0([1 end],:,:, :)=nan; u0=u0(:);
229 i=find(~isnan(u0));
230 nJ=length(i);
231 Jac=nan(nJ);
232 for j=1:nJ
233     u0(i)=((1:nJ)==j);
234     dudt=patchSys1(0,u0);
235     Jac(:,j)=dudt(i);
236 end
237 nonSymmetric=norm(Jac-Jac')
238 assert(nonSymmetric<5e-9,'failed symmetry')
239 Jac(abs(Jac)<1e-12)=0;

```

Find the eigenvalues of the Jacobian, and list for inspection in [Table 3.1](#): the spectral interpolation is effectively exact for the macroscale; quadratic interpolation is usually quantitatively in error; quartic interpolation appears to be the lowest order for reliable quantitative accuracy.

The number of zero eigenvalues, $nZeroEv$, indicates the number of decoupled systems in this patch configuration.

Table 3.1: example parameters and list of eigenvalues (every fourth one listed is sufficient due to symmetry): `nPatch = 19`, `ratio = 0.1`, `nSubP = 5`. The columns are for various `ordCC`, in order: 0, spectral interpolation; 2, quadratic; 4, quartic; and 6, sixth order.

```

cHetr =
    6.9617
    0.4217
    2.0624
leadingEvals =
    2e-11      -2e-12      4e-12      -2e-11
    -0.9999     -1.5195     -1.0127     -1.0003
    -3.9992     -11.861     -4.7785     -4.0738
    -8.9960     -45.239     -17.164     -10.703
    -15.987     -116.27     -56.220     -30.402
    -24.969     -230.63     -151.74     -92.830
    -35.936     -378.80     -327.36     -247.37
    -48.882     -535.89     -570.87     -521.89
    -63.799     -668.21     -818.33     -855.72
    -80.678     -743.96     -976.57     -1093.4
    -29129      -29233      -29227      -29222
    -29151      -29234      -29229      -29223

280 [evecs,evals]=eig(Jac);
281 eval=-sort(-diag(real(evals)));
282 nZeroEv=sum(eval(:)>-1e-5)
283 leadingEvals=[leadingEvals eval(1:3*nPatch)];
284 % leadingEvals=[leadingEvals eval([1, (nZeroEv+1):2:(nZeroEv*nPatch+4)])];

End of the for-loop over orders of interpolation, and output the tables of
eigenvalues.

291 end
292 disp(' spectral     quadratic      quartic   sixth-order ...')
293 leadingEvals=leadingEvals

End of the main script.

```

3.5.2 `heteroDiff()`: heterogeneous diffusion

This function codes the lattice heterogeneous diffusion inside the patches. For 2D input arrays `u` and `x` (via edge-value interpolation of `patchSys1`, [Section 3.2](#)), computes the time derivative [\(3.1\)](#) at each point in the interior of a patch, output in `ut`. The column vector of diffusivities c_i , and possibly Burgers' advection coefficients b_i , have previously been stored in struct `patches.cs`.

```

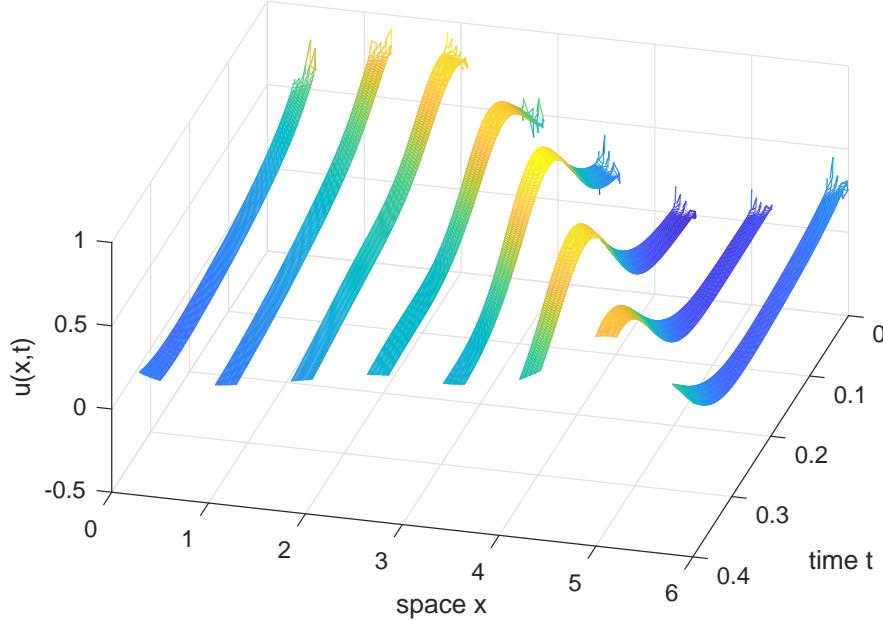
21 function ut = heteroDiff(t,u,patches)
22 dx = diff(patches.x(2:3)); % space step
23 i = 2:size(u,1)-1; % interior points in a patch

```

```
24 ut = nan+u; % preallocate output array
25 ut(:,:, :) = diff(patches.cs(:,1,:).*diff(u))/dx^2;
26 % possibly include heterogeneous Burgers' advection
27 if size(patches.cs,2)>1 % check for advection coeffs
28     buu = patches.cs(:,2,:).*u.^2;
29     ut(:,:, :) = ut(:,:, :) - (buu(:,:,i+1,:)-buu(:,:,i-1,:))/(dx*2);
30 end
31 end% function
```

Fin.

Figure 3.8: a short time simulation of the Burgers' map (Section 3.6.3) on patches in space. It requires many very small time-steps only just visible in this mesh.



3.6 BurgersExample: simulate Burgers' PDE on patches

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[Figure 3.2](#) shows a previous example simulation in time generated by the patch scheme applied to Burgers' PDE. The code in the example of this section similarly applies the patch scheme to a microscale space-time map ([Figure 3.8](#)), a map derived as a microscale space-time discretisation of Burgers' PDE. Then this example applies projective integration to simulate further in time.

3.6.1 Script code to simulate a microscale space-time map

This first part of the script implements the following patch/gap-tooth scheme (left-right arrows denote function recursion).

1. configPatches1
2. burgerBurst \mapsto patchSys1 \mapsto burgersMap
3. process results

Establish global data struct for the microscale Burgers' map ([Section 3.6.3](#)) solved on 2π -periodic domain, with eight patches, each patch of half-size ratio 0.2, with seven points within each patch, and say fourth-order interpolation provides edge-values that couple the patches.

```

50 global patches
51 nPatch = 8
52 ratio = 0.2
53 nSubP = 7
54 interpOrd = 4
55 Len = 2*pi
56 configPatches1(@burgersMap,[0 Len],nan,nPatch,interpOrd,ratio,nSubP);

```

Set an initial condition, and simulate a burst of the microscale space-time map over a time 0.2 using the function `burgerBurst()` ([Section 3.6.4](#)).

```

64 u0 = 0.4*(1+sin(patches.x))+0.1*randn(size(patches.x));
65 [ts,us] = burgersBurst(0,u0,0.4);

```

Plot the simulation. Use only the microscale values interior to the patches by setting the edges to `nan` in order to leave gaps.

```

73 figure(1),clf
74 xs = patches.x; xs([1 end],:) = nan;
75 mesh(ts,xs(:,us'))
76 xlabel('time $t$'), ylabel('space $x$'), zlabel('$u(x,t)$')
77 view(105,45)

```

Save the plot to file to form [Figure 3.8](#).

```
83 if0urCf2eps([mfilename 'MapU'])
```

3.6.2 Alternatively use projective integration

Around the microscale burst `burgerBurst()`, wrap the projective integration function `PIRK2()` of [Section 2.2](#). [Figure 3.9](#) shows the resultant macroscale prediction of the patch centre values on macroscale time-steps.

This second part of the script implements the following design.

1. `configPatches1` (done in [Section 3.6.1](#))
2. `PIRK2` \mapsto `burgerBurst` \mapsto `patchSys1` \mapsto `burgersMap`
3. process results

Mark that edge-values of patches are not to be used in the projective extrapolation by setting initial values to NaN.

```
115 u0([1 end],:) = nan;
```

Set the desired macroscale time-steps, and microscale burst length over the time domain. Then projectively integrate in time using `PIRK2()` which is second-order accurate in the macroscale time-step.

```

124 ts = linspace(0,0.5,11);
125 bT = 3*(ratio*Len/nPatch/(nSubP/2-1))^2

```

Figure 3.9: macroscale space-time field $u(x, t)$ in a basic projective integration of the patch scheme applied to the microscale Burgers' map.

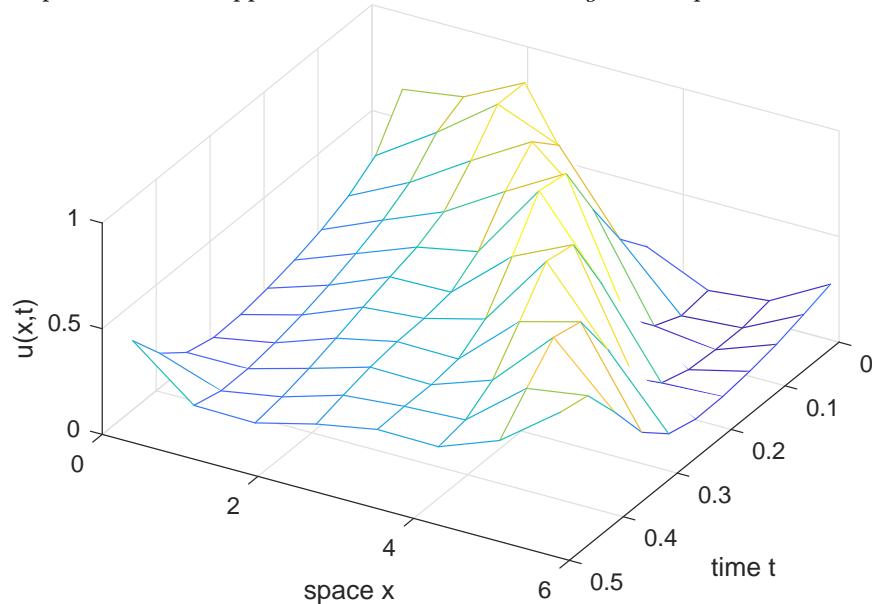
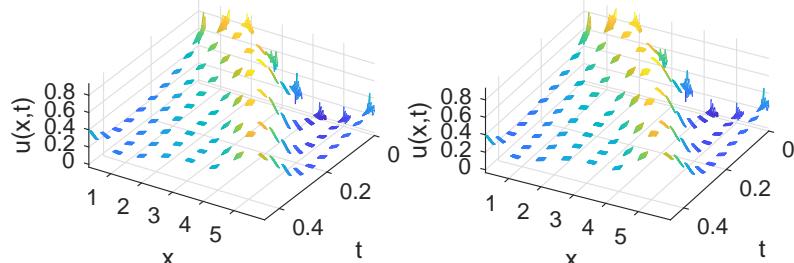


Figure 3.10: the microscale field $u(x, t)$ during each of the microscale bursts used in the projective integration. View this stereo pair cross-eyed.



```

126 addpath('..../ProjInt')
127 [us,tss,uss] = PIRK2(@burgersBurst,ts,u0(:,bT));

```

Plot and save the macroscale predictions of the mid-patch values to give the macroscale mesh-surface of Figure 3.9 that shows a progressing wave solution.

```

135 figure(2),clf
136 midP = (nSubP+1)/2;
137 mesh(ts,xs(midP,:),us(:,midP:nSubP:end)')
138 xlabel('time $t$'), ylabel('space $x$'), zlabel('$u(x,t)$')
139 view(120,50)
140 ifOurCf2eps([mfilename 'U'])

```

Then plot and save the microscale mesh of the microscale bursts shown in Figure 3.10 (a stereo pair). The details of the fine microscale mesh are almost invisible.

```

155 figure(3),clf
156 for k = 1:2, subplot(2,2,k)

```

```

157     mesh(tss, xs(:, uss'))
158     ylabel('space $x$'), xlabel('time $t$'), zlabel('$u(x,t)$')
159     axis tight, view(126-4*k, 50)
160 end
161 ifOutCf2eps([mfilename 'Micro'])

```

3.6.3 burgersMap(): discretise the PDE microscale

This function codes the microscale Euler integration map of the lattice differential equations inside the patches. Only the patch-interior values are mapped (`patchSys1()` overrides the edge-values anyway).

```

13 function u = burgersMap(t, u, patches)
14     u = squeeze(u);
15     dx = diff(patches.x(2:3));
16     dt = dx^2/2;
17     i = 2:size(u,1)-1;
18     u(i,:) = u(i,:) + dt*( diff(u,2)/dx^2 ...
19         -20*u(i,:).*(u(i+1,:)-u(i-1,:))/(2*dx) );
20 end

```

3.6.4 burgerBurst(): code a burst of the patch map

```
10 function [ts, us] = burgersBurst(ti, ui, bT)
```

First find and set the number of microscale time-steps.

```

16 global patches
17 dt = diff(patches.x(2:3))^2/2;
18 ndt = ceil(bT/dt - 0.2);
19 ts = ti+(0:ndt)*dt;

```

Use `patchSys1()` (Section 3.2) to apply the microscale map over all time-steps in the burst. The `patchSys1()` interface provides the interpolated edge-values of each patch. Store the results in rows to be consistent with ODE and projective integrators.

```

29 us = nan(ndt+1, numel(ui));
30 us(1,:) = reshape(ui, 1, []);
31 for j = 1:ndt
32     ui = patchSys1(ts(j), ui);
33     us(j+1,:) = reshape(ui, 1, []);
34 end

```

Linearly interpolate (extrapolate) to get the field values at the precise final time of the burst. Then return.

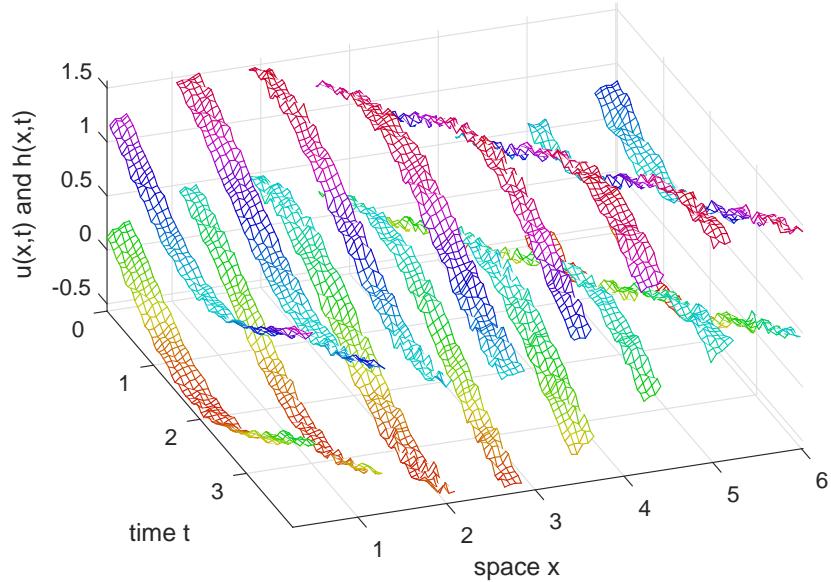
```

41 ts(ndt+1) = ti+bT;
42 us(ndt+1,:) = us(ndt,:) ...
43     + diff(ts(ndt:ndt+1))/dt*diff(us(ndt:ndt+1,:));
44 end

```

Fin.

Figure 3.11: water depth $h(x, t)$ (above) and velocity field $u(x, t)$ (below) of the gap-tooth scheme applied to the ideal linear wave PDE (3.3) with $f_1 = f_2 = 0$. The microscale random component to the initial condition persists in the simulation—but the macroscale wave still propagates.



3.7 waterWaveExample: simulate a water wave PDE on patches

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3.7.3	waterWavePDE(): water wave PDE	91

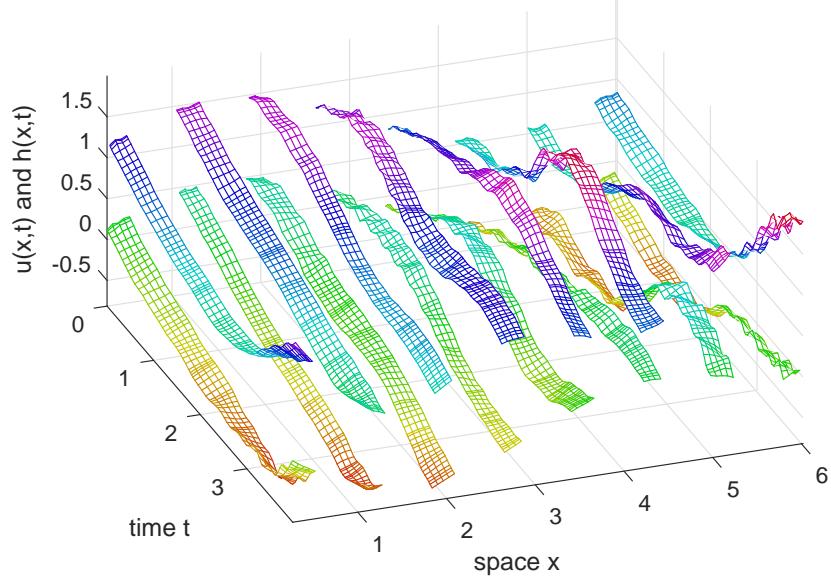
Figure 3.11 shows an example simulation in time generated by the patch scheme applied to an ideal wave PDE (Cao & Roberts 2013). The inter-patch coupling is realised by spectral interpolation of the mid-patch values to the patch edges.

This approach, based upon the differential equations coded in Section 3.7.2, may be adapted by a user to a wide variety of 1D wave and wave-like systems. For example, the differential equations of Section 3.7.3 that describe the nonlinear microscale simulator of the nonlinear shallow water wave PDE derived from the Smagorinski model of turbulent flow (Cao & Roberts 2012, 2016a).

Often, wave-like systems are written in terms of two conjugate variables, for example, position and momentum density, electric and magnetic fields, and water depth $h(x, t)$ and mean longitudinal velocity $u(x, t)$ as herein. The approach developed in this section applies to any wave-like system in the form

$$\frac{\partial h}{\partial t} = -c_1 \frac{\partial u}{\partial x} + f_1[h, u] \quad \text{and} \quad \frac{\partial u}{\partial t} = -c_2 \frac{\partial h}{\partial x} + f_2[h, u], \quad (3.3)$$

Figure 3.12: water depth $h(x, t)$ (above) and velocity field $u(x, t)$ (below) of the gap-tooth scheme applied to the Smagorinski shallow water wave PDEs (3.4). The microscale random initial component decays where the water speed is non-zero due to ‘turbulent’ dissipation.



where the brackets indicate that the two nonlinear functions f_1 and f_2 may involve various spatial derivatives of the fields $h(x, t)$ and $u(x, t)$. For example, Section 3.7.3 encodes a nonlinear Smagorinski model of turbulent shallow water (Cao & Roberts 2012, 2016a, e.g.) along an inclined flat bed: let x measure position along the bed and in terms of fluid depth $h(x, t)$ and depth-averaged longitudinal velocity $u(x, t)$ the model PDEs are

$$\frac{\partial h}{\partial t} = -\frac{\partial(hu)}{\partial x}, \quad (3.4a)$$

$$\frac{\partial u}{\partial t} = 0.985 \left(\tan \theta - \frac{\partial h}{\partial x} \right) - 0.003 \frac{u|u|}{h} - 1.045u \frac{\partial u}{\partial x} + 0.26h|u| \frac{\partial^2 u}{\partial x^2}, \quad (3.4b)$$

where $\tan \theta$ is the slope of the bed. The PDE (3.4a) represents conservation of the fluid. The momentum PDE (3.4b) represents the effects of turbulent bed drag $u|u|/h$, self-advection $u\partial u/\partial x$, nonlinear turbulent dispersion $h|u|\partial^2 u/\partial x^2$, and gravitational hydrostatic forcing ($\tan \theta - \partial h/\partial x$). Figure 3.12 shows one simulation of this system—for the same initial condition as Figure 3.11.

For such wave-like systems, let’s implement both a staggered microscale grid and also staggered macroscale patches, as introduced by Cao & Roberts (2016b) in their Figures 3 and 4, respectively.

3.7.1 Script code to simulate wave systems

This example script implements the following patch/gap-tooth scheme (left-right arrows denote function recursion).

1. configPatches1, and add micro-information

-
2. `ode15s` \mapsto `patchSys1` \mapsto `idealWavePDE`
 3. process results
 4. `ode15s` \mapsto `patchSys1` \mapsto `waterWavePDE`
 5. process results

Establish the global data struct `patches` for the PDES (3.3) (linearised) solved on 2π -periodic domain, with eight patches, each patch of half-size ratio 0.2, with eleven micro-grid points within each patch, and spectral interpolation (-1) of ‘staggered’ macroscale patches to provide the edge-values of the inter-patch coupling conditions.

```

119 global patches
120 nPatch = 8
121 ratio = 0.2
122 nSubP = 11 %of the form 4*n-1
123 Len = 2*pi;
124 configPatches1(@idealWavePDE,[0 Len],nan,nPatch,-1,ratio,nSubP);

```

Identify which micro-grid points are h or u values on the staggered micro-grid. Also store the information in the struct `patches` for use by the time derivative function.

```

134 uPts = mod( (1:nSubP)' + (1:nPatch) ,2);
135 hPts = find(uPts==0);
136 uPts = find(uPts==1);
137 patches.hPts = hPts; patches.uPts = uPts;

```

Set an initial condition of a progressive wave, and check evaluation of the time derivative. The capital letter U denotes an array of values merged from both u and h fields on the staggered grids (here with some optional microscale wave noise).

```

148 U0 = nan(nSubP,nPatch);
149 U0(hPts) = 1+0.5*sin(patches.x(hPts));
150 U0(uPts) = 0+0.5*sin(patches.x(uPts));
151 U0 = U0+0.02*randn(nSubP,nPatch);

```

Conventional integration in time Integrate in time using standard MATLAB/Octave stiff integrators. Here do the two cases of the ideal wave and the water wave equations in the one loop.

```

161 for k = 1:2

```

When using `ode15s/lsode` we subsample the results because micro-grid scale waves do not dissipate and so the integrator takes very small time-steps for all time.

```

169 if ~exist('OCTAVE_VERSION','builtin')
170     [ts,Ucts] = ode15s( @patchSys1,[0 4],U0(:));
171     ts = ts(1:5:end);
172     Ucts = Ucts(1:5:end,:);
173 else % octave version is slower

```

```

174     [ts,Ucts] = odeOcts(@patchSys1,[0 4],U0(:));
175 end

```

Plot the simulation.

```

181 figure(k),clf
182 xs = squeeze(patches.x); xs([1 end],:) = nan;
183 mesh(ts,xs(hPts),Ucts(:,hPts)'),hold on
184 mesh(ts,xs(uPts),Ucts(:,uPts)'),hold off
185 xlabel('time $t$'), ylabel('space $x$'), zlabel('$u(x,t)$ and $h(x,t)$')
186 axis tight, view(70,45)

```

Optionally save the plot to file.

```

192 if0urCf2eps([mfilename num2str(k) 'CtsUH'])

```

For the second time through the loop, change to the Smagorinski turbulence model (3.4) of shallow water flow, keeping other parameters and the initial condition the same.

```

202 patches.fun = @waterWavePDE;
203 end

```

Could use projective integration As yet a simple implementation appears to fail, so it needs more exploration and thought. End of the main script.

3.7.2 idealWavePDE(): ideal wave PDE

This function codes the staggered lattice equation inside the patches for the ideal wave PDE system $h_t = -u_x$ and $u_t = -h_x$. Here code for a staggered micro-grid, index i , of staggered macroscale patches, index j : the array

$$U_{ij} = \begin{cases} u_{ij} & i + j \text{ even}, \\ h_{ij} & i + j \text{ odd}. \end{cases}$$

The output **Ut** contains the merged time derivatives of the two staggered fields. So set the micro-grid spacing and reserve space for time derivatives.

```

24 function Ut = idealWavePDE(t,U,patches)
25 dx = diff(patches.x(2:3));
26 U = squeeze(U);
27 Ut = nan(size(U)); ht = Ut;

```

Compute the PDE derivatives only at interior micro-grid points of the patches.

```

34 i = 2:size(U,1)-1;

```

Here ‘wastefully’ compute time derivatives for both PDEs at all grid points—for simplicity—and then merge the staggered results. Since $\dot{h}_{ij} \approx -(u_{i+1,j} - u_{i-1,j})/(2 \cdot dx) = -(U_{i+1,j} - U_{i-1,j})/(2 \cdot dx)$ as adding/subtracting one from the index of a h -value is the location of the neighbouring u -value on the staggered micro-grid.

```

46 ht(i,:) = -(U(i+1,:)-U(i-1,:))/(2*dx);

```

Since $\dot{u}_{ij} \approx -(h_{i+1,j} - h_{i-1,j})/(2 \cdot dx) = -(U_{i+1,j} - U_{i-1,j})/(2 \cdot dx)$ as adding/subtracting one from the index of a u -value is the location of the neighbouring h -value on the staggered micro-grid.

```
56 Ut(i,:) = -(U(i+1,:)-U(i-1,:))/(2*dx);
```

Then overwrite the unwanted \dot{u}_{ij} with the corresponding wanted \dot{h}_{ij} .

```
63 Ut(patches.hPts) = ht(patches.hPts);
64 end
```

3.7.3 waterWavePDE(): water wave PDE

This function codes the staggered lattice equation inside the patches for the nonlinear wave-like PDE system (3.4). Also, regularise the absolute value appearing the the PDEs via the one-line function `rabs()`.

```
16 function Ut = waterWavePDE(t,U,patches)
17 rabs = @(u) sqrt(1e-4 + u.^2);
```

As before, set the micro-grid spacing, reserve space for time derivatives, and index the patch-interior points of the micro-grid.

```
25 dx = diff(patches.x(2:3));
26 U = squeeze(U);
27 Ut = nan(size(U)); ht = Ut;
28 i = 2:size(U,1)-1;
```

Need to estimate h at all the u -points, so into V use averages, and linear extrapolation to patch-edges.

```
36 ii = i(2:end-1);
37 V = Ut;
38 V(ii,:) = (U(ii+1,:)+U(ii-1,:))/2;
39 V(1:2,:) = 2*U(2:3,:)-V(3:4,:);
40 V(end-1:end,:) = 2*U(end-2:end-1,:)-V(end-3:end-2,:);
```

Then estimate $\partial(hu)/\partial x$ from u and the interpolated h at the neighbouring micro-grid points.

```
47 ht(i,:) = -(U(i+1,:).*V(i+1,:)-U(i-1,:).*V(i-1,:))/(2*dx);
```

Correspondingly estimate the terms in the momentum PDE: u -values in U_i and $V_{i\pm 1}$; and h -values in V_i and $U_{i\pm 1}$.

```
55 Ut(i,:) = -0.985*(U(i+1,:)-U(i-1,:))/(2*dx) ...
56 -0.003*U(i,:).*rabs(U(i,:)./V(i,:)) ...
57 -1.045*U(i,:).*(V(i+1,:)-V(i-1,:))/(2*dx) ...
58 +0.26*rabs(V(i,:).*U(i,:)).*(V(i+1,:)-2*U(i,:)+V(i-1,:))/dx^2/2;
```

where the mysterious division by two in the second derivative is due to using the averaged values of u in the estimate:

$$\begin{aligned}
 u_{xx} &\approx \frac{1}{4\delta^2}(u_{i-2} - 2u_i + u_{i+2}) \\
 &= \frac{1}{4\delta^2}(u_{i-2} + u_i - 4u_i + u_i + u_{i+2}) \\
 &= \frac{1}{2\delta^2} \left(\frac{u_{i-2} + u_i}{2} - 2u_i + \frac{u_i + u_{i+2}}{2} \right) \\
 &= \frac{1}{2\delta^2} (\bar{u}_{i-1} - 2u_i + \bar{u}_{i+1}).
 \end{aligned}$$

Then overwrite the unwanted \dot{u}_{ij} with the corresponding wanted \dot{h}_{ij} .

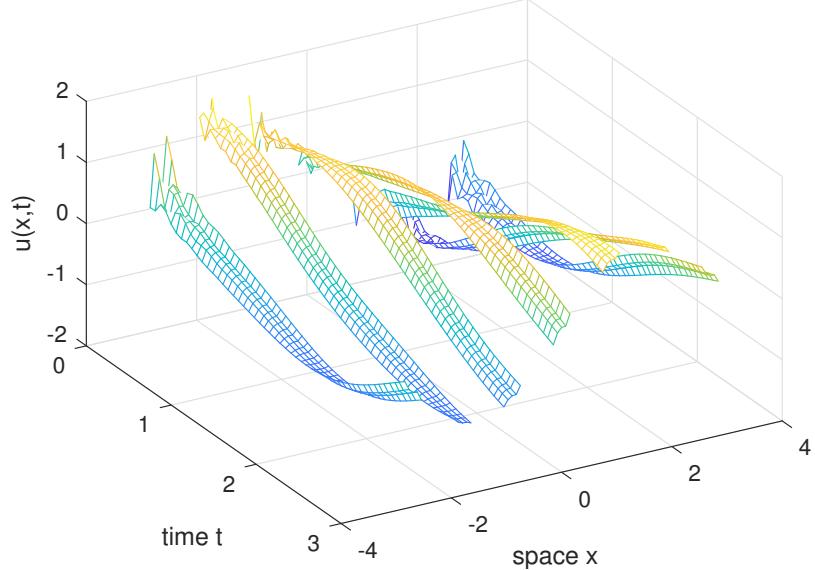
```

74     Ut(patches.hPts) = ht(patches.hPts);
75   end

```

Fin.

Figure 3.13: wave field $u(x, t)$ of the gap-tooth scheme applied to the weakly damped wave (3.5). The microscale random component to the initial condition persists in the simulation until the weak damping smooths the sub-patch fluctuations—but the macroscale wave still propagates.



3.8 homoWaveEdgy1: computational homogenisation of a 1D wave by simulation on small patches

[Figure 3.13](#) shows an example simulation in time generated by the patch scheme applied to macroscale wave propagation through a medium with microscale heterogeneity. The inter-patch coupling is realised by spectral interpolation of the patch's next-to-edge values to the patch opposite edges. This coupling preserves symmetry in many systems.

Often, wave-like systems are written in terms of two conjugate variables, for example, position and momentum density, electric and magnetic fields, and water depth and mean longitudinal velocity. Here suppose the spatial microscale lattice is at points x_i , with constant spacing dx . With dependent variables $u_i(t)$ and $v_i(t)$, simulate the microscale lattice, weakly damped, wave system

$$\frac{\partial u_i}{\partial t} = v_i, \quad \frac{\partial v_i}{\partial t} = \frac{1}{dx^2} \delta[c_{i-1/2} \delta u_i] + \frac{0.02}{dx^2} \delta^2 v_i, \quad (3.5)$$

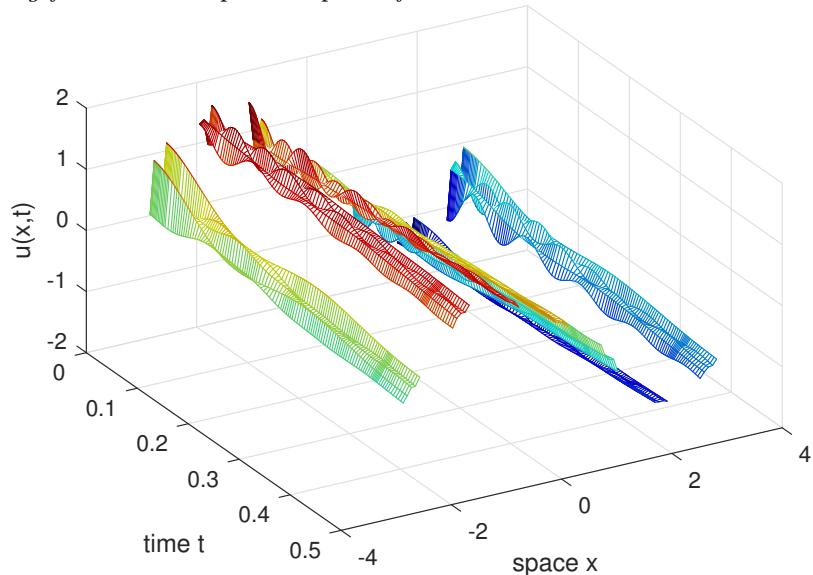
in terms of the centred difference operator δ . The system has a microscale heterogeneity via the coefficients $c_{i+1/2}$ which we assume to have some given known periodicity. [Figure 3.13](#) shows one patch simulation of this system: observe the effects of the heterogeneity within each patch.

3.8.1 Script code to simulate heterogeneous wave systems

This example script implements the following patch/gap-tooth scheme (left-right arrows denote function recursion).

1. configPatches1, and add micro-information

Figure 3.14: wave field $u(x, t)$ of the gap-tooth scheme applied to the weakly damped wave (3.5). Over this shorter meso-time we see the macroscale wave emerging from the damped sub-patch fast waves.



2. `ode15s` \mapsto `patchSys1` \mapsto `heteroWave`
3. plot the simulation
4. use `patchSys1` to check the Jacobian

First establish the microscale heterogeneity has micro-period `mPeriod` on the lattice, and random log-normal values, albeit normalised to have harmonic mean one. This normalisation then means that macroscale waves on a domain of length 2π have near integer frequencies, 1, 2, 3, Then the heterogeneity is to be repeated `nPeriodsPatch` times within each patch.

```

91 mPeriod = 3
92 cHetr = exp(1*randn(mPeriod,1));
93 cHetr = cHetr*mean(1./cHetr) % normalise
94 nPeriodsPatch=1

```

Establish the global data struct `patches` for the microscale heterogeneous lattice wave system (3.5) solved on 2π -periodic domain, with seven patches, here each patch of size ratio 0.25 from one side to the other, with five micro-grid points in each patch, and spectral interpolation (0) to provide the edge-values of the inter-patch coupling conditions. Setting `patches.EdgeyInt` to one means the edge-values come from interpolating the opposite next-to-edge values of the patches (not the mid-patch values).

```

111 global patches
112 nPatch = 7
113 ratio = 0.25
114 nSubP = nPeriodsPatch*mPeriod+2
115 configPatches1(@heteroWave, [-pi pi], nan, nPatch ...
116 , 0, ratio, nSubP, 'EdgeyInt', true, 'hetCoeffs', cHetr);

```

Simulate Set the initial conditions of a simulation to be that of a macroscopic progressive wave, via sin / cos, perturbed by significant random microscale noise, via randn.

```
128 uv0(:,1,1,:) = -sin(patches.x)+0.3*randn(nSubP,1,1,nPatch);
129 uv0(:,2,1,:) = +cos(patches.x)+0.3*randn(nSubP,1,1,nPatch);
```

Integrate for about half a wave period using standard stiff integrators (which do not work efficiently until after the fast waves have decayed).

```
137 if ~exist('OCTAVE_VERSION','builtin')
138     [ts,us] = ode15s(@patchSys1, [0 3], uv0(:));
139 else % octave version
140     [ts,us] = odeOcts(@patchSys1, [0 3], uv0(:));
141 end
```

Plot space-time surface of the simulation We want to see the edge values of the patches, so we 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.

```
153 xs = squeeze(patches.x);
154 us = patchEdgeInt1( permute( reshape(us,length(ts) ...
155 ,nSubP,2,nPatch) ,[2 3 1 4]) );
156 xs(end+1,:) = nan; us(end+1,:,:,:) = nan;
157 us = reshape(permute(us,[1 4 2 3]),length(xs(:)),2,[]);
```

Now plot two space-time graphs. The first is every time step over a meso-time to see the oscillation and decay of the fast sub-patch waves. The second is subsampled surface over the macroscale duration of the simulation to show the propagation of the macroscale wave over the heterogeneous lattice.

```
169 for p=1:2
170     switch p
171         case 1, j=find(ts<0.5);
172         case 2, [~,j]=min(abs(ts-linspace(ts(1),ts(end),50)));
173     end
174     figure(p),clf
175     mesh(ts(j),xs(:,1,j)), view(60,40)
176     xlabel('time $t$'), ylabel('space $x$'), zlabel('$u(x,t)$')
177     ifOutCf2eps([mfilename 'U' num2str(p)])
178 end
```

Compute Jacobian and its spectrum Form the Jacobian matrix, 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 systems variables.

```
190 u0=repmat(0*patches.x,1,2); u0([1 end],:) = nan; u0=u0(:);
191 i=find(~isnan(u0));
192 nJ=length(i);
193 Jac=nan(nJ);
```

Table 3.2: example parameters and list of eigenvalues (every fourth one listed is sufficient due to symmetry): `nPatch = 7`, `ratio = 0.25`, `nSubP = 5`. The spectrum is satisfactory for weakly damped macroscale waves, and medium-damped microscale sub-patch fast waves.

```
cHetr =
    0.58459
    1.0026
    3.4253
eval =
    2.2701e-16 + 1.4225e-07i
    -0.013349 + 0.99941i
    -0.053324 + 1.9952i
    -0.11971 + 2.9838i
    -5.1527 + 19.554i
    -5.2679 + 19.695i
    -5.3383 + 19.779i
    -5.3619 + 36.632i
    -5.3722 + 36.632i
    -5.4026 + 36.631i
    -5.4514 + 36.63i
```

```
194 for j=1:nJ
195     u0(i)=((1:nJ)==j);
196     dudt=patchSys1(0,u0);
197     Jac(:,j)=dudt(i);
198 end
199 Jac(abs(Jac)<1e-12)=0;
```

Find the eigenvalues of the Jacobian, and list for inspection in [Table 3.2](#).

```
231 [evecs,evals]=eig(Jac);
232 eval=sort(diag(evals));
233 slowestEvals=eval(2:4:4*nPatch)
```

End of the main script.

3.8.2 `heteroWave()`: wave in heterogeneous media with weak viscous damping

This function codes the lattice heterogeneous wave equation, with weak viscosity, inside the patches. For 3D input array \mathbf{u} ($u_{ij} = \mathbf{u}(i,1,j)$ and $v_{ij} = \mathbf{u}(i,2,j)$) and 2D array \mathbf{x} (obtained in full via edge-value interpolation of `patchSys1`, [Section 3.2](#)), computes the time derivatives at each point in the interior of a patch, output in \mathbf{ut} :

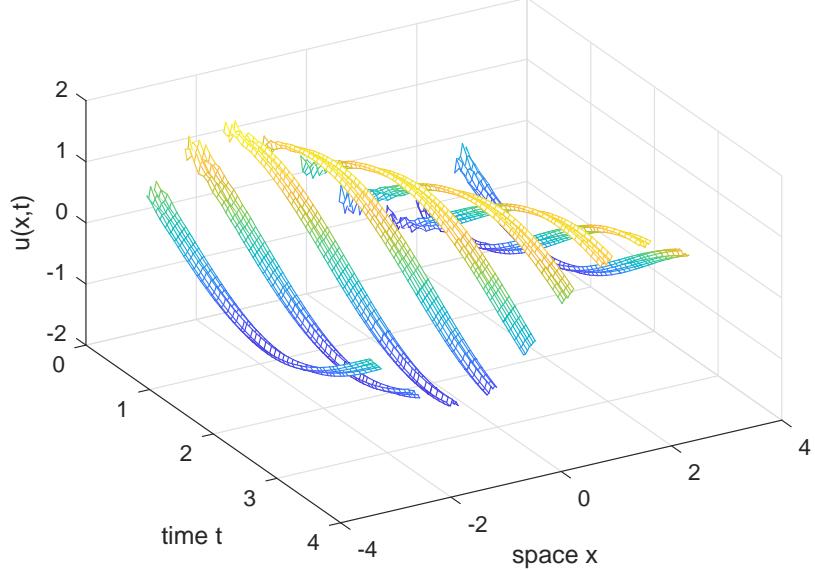
$$\frac{\partial u_{ij}}{\partial t} = v_{ij}, \quad \frac{\partial v_{ij}}{\partial t} = \frac{1}{dx^2} \delta[c_{i-1/2} \delta u_{ij}] + \frac{0.02}{dx^2} \delta^2 v_{ij}.$$

The column vector (or possibly array) of diffusion coefficients c_i have previously been stored in struct `patches`.

```
27 function ut = heteroWave(t,u,patches)
28 u = squeeze(u);
29 dx = diff(patches.x(2:3)); % space step
30 i = 2:size(u,1)-1; % interior points in a patch
31 ut = nan(size(u)); % preallocate output array
32 ut(i,1,:) = u(i,2,:); % du/dt=v then dvdt=
33 ut(i,2,:) = diff(patches.cs.*diff(u(:,1,:)))/dx^2 ...
            +0.02*diff(u(:,2,:),2)/dx^2;
34 end% function
```

Fin.

Figure 3.15: wave field $u(x, t)$ of the gap-tooth scheme applied to the wave (3.6). The microscale random component to the initial condition, the sub-patch fluctuations, decays, leaving the emergent macroscale wave in the heterogeneous media. This simulation uses nine patches of ‘large’ size ratio 0.25 for visibility.



3.9 waveEdgy1: simulate a 1D, first-order, wave PDE on small patches

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Figure 3.15 shows an example simulation in time generated by the patch scheme applied to macroscale diffusion propagation through a medium with microscale heterogeneity. The inter-patch coupling is realised by spectral interpolation of the patch’s next-to-edge values to the patch opposite edges. Such coupling preserves symmetry in many systems, and in this first-order wave PDE preserves skew-symmetry.

The first-order wave-like PDE is $u_t = -\frac{1}{2}(cu)_x - \frac{1}{2}cu_x$, which when c is constant becomes the canonical first-order wave PDE $u_t = -cu_x$. The differential operator on the right-hand side is skew-symmetric: letting $\mathcal{D} = -\frac{1}{2}(c\cdot)_x - \frac{1}{2}c\partial_x$ then $\int v\mathcal{D}u dx = \int -v(cu)_x - v\frac{1}{2}cu_x dx = -\int \frac{1}{2}v_x cu + \frac{1}{2}(vc)_x u dx = -\int u\mathcal{D}v dx$.

To discretise in space, suppose the spatial microscale lattice is at points x_i , with constant spacing d . With dependent variables $u_i(t)$, simulate the microscale lattice, in terms of the centred difference δ and mean μ , wave system

$$\frac{du_i}{dt} = -\frac{1}{2d} [\delta(c_i \mu u_i) + \mu(c_i \delta u_i)] = -\frac{1}{2d} \left[c_{i+\frac{1}{2}} u_{i+1} - c_{i-\frac{1}{2}} u_{i-1} \right]. \quad (3.6)$$

[Figure 3.15](#) shows one patch simulation of this space-time system, except it also includes a $\nu = 0.001$ small ‘viscous’ dissipation, $\nu\delta^2u_i/d^2$, to weakly damp the microscale, sub-patch, fast waves.

3.9.1 Script code to simulate heterogeneous wave systems

This example script implements the following patch/gap-tooth scheme (left-right arrows denote function recursion).

1. configPatches1, and add micro-information
2. ode15s \rightarrow patchSys1 \rightarrow waveFirst
3. plot the simulation
4. use patchSys1 to explore the Jacobian

First establish the microscale heterogeneity has (odd-valued) micro-period `mPeriod` on the lattice, and random log-normal values, normalised. This normalisation means that macroscale wave on a domain of length 2π should have nearly integer frequencies, 0, 1, 2, . . .—except that the normalisation is exact only for periods 3 and 5. Then the heterogeneity is repeated `nPeriodsPatch` times within each patch.

```

89 mPeriod = 5 % needs to be odd for a wave
90 cHetr = exp(0.1*randn(mPeriod,1)); % 0.3 appears max reasonable
91 if mPeriod==3,
92     cHetr=cHetr*mean(cHetr.^2)/prod(cHetr) % normalise
93 elseif mPeriod==5,
94     cHetr=cHetr*mean(cHetr.^2.*cHetr([3 4 5 1 2]).^2)/prod(cHetr)
95 else cHetr=cHetr*mean(1./cHetr) % roughly normalise
96 end
97 nPeriodsPatch=1 % also needs to be odd

```

Establish the global data struct `patches` for the microscale heterogeneous lattice wave system [\(3.6\)](#) solved on 2π -periodic domain, with nine patches, here each patch of size ratio 0.25 from one side to the other, with five micro-grid points in each patch, and quartic interpolation (4) to provide the edge-values via the inter-patch coupling conditions. Setting `EdgyInt` to

- true means the edge-values come from interpolating the opposite next-to-edge values of the patches (not the mid-patch values); whereas
- false means the time integration appears OK, but the Jacobian is, correctly, not skew-symmetric for this case of interpolating mid-patch values.

```

120 global patches
121 nPatch = 9
122 ratio = 0.25
123 EdgyInt=true
124 nPeriodsPatch = (2-EdgyInt)*nPeriodsPatch;
125 nSubP = nPeriodsPatch*mPeriod+1+EdgyInt
126 configPatches1(@waveFirst, [-pi pi], nan, nPatch, 4 ...
    ,ratio,nSubP,'EdgyInt',EdgyInt,'hetCoeffs',cHetr);

```

Specify the weak damping of the sub-patch, fast, microscale waves.

```
135 patches.nu=0.003;
```

Simulate Set the initial conditions of a simulation to be that of a sine wave perturbed by significant random microscale noise, via `randn`.

```
145 xs=squeeze(patches.x);
146 u0 = -sin(xs)+0.1*randn(nSubP,nPatch);
```

Integrate using standard stiff integrators.

```
152 if ~exist('OCTAVE_VERSION','builtin')
153     [ts,us] = ode23(@patchSys1, [0 3.5], u0(:));
154 else % octave version
155     [ts,us] = odeOcts(@patchSys1, [0 0.5], u0(:));
156 end
```

Plot space-time surface of the simulation Let's see the edge values of the patches. For the field values (which are rows in `us`) we need to reshape, permute, interpolate with `patchEdgeInt1` to get edge values, pad with `nans`, and reshape again.

```
167 xs(end+1,:) = nan;
168 us = patchEdgeInt1( permute( reshape(us ...
169     ,length(ts),nSubP,nPatch) ,[2 1 3]) );
170 us(end+1,:,:,:)= nan;
171 us=reshape(permute(squeeze(us),[1 3 2]),[],length(ts));
```

Now plot a space-time graph. Subsample the data over the macroscale duration of the simulation to show the propagation of the macroscale wave over the heterogeneous lattice.

```
181 [~,j]=min(abs(ts-linspace(ts(1),ts(end),50)));
182 figure(1),clf
183 mesh(ts(j),xs(:,us(:,j))), view(60,40)
184 xlabel('time $t$'), ylabel('space $x$'), zlabel('$u(x,t)$')
185 if0urCf2eps([mfilename 'U' num2str(2)])
```

Compute Jacobian and its spectrum Let's explore the Jacobian dynamics for a range of orders of interpolation, all for the same patch design and heterogeneity. Here use a smaller ratio, and more patches, as we do not plot. Set the weak damping to zero so we explore the ideal case of the wave system (3.6).

```
198 ratio=0.01
199 nPatch=19
200 leadingFreqs=[];
201 for ord=0:2:8
202     ordInterp=ord
203     configPatches1(@waveFirst,[-pi pi],nan,nPatch,ord ...
```

Table 3.3: example parameters and list of eigenvalues (every second one listed is sufficient due to symmetry): `nPatch = 19`, `ratio = 0.03`, `nSubP = 7`. The columns are for various `ordCC`, in order: 0, spectral interpolation; 2, quadratic; 4, quartic; and 6, sixth order. Rows are ordered in the effective wavenumber of the corresponding eigenvector (the number of zero crossings).

```
cHetr =
    0.6614
    1.5758
    1.8645
    1.4600
    0.8486
leadingFreqs =
    0      0      0      0
    1.0000  0.9819  0.9996  1.0000
    2.0000  1.8574  1.9879  1.9989
    2.9999  2.5318  2.9138  2.9830
    3.9997  2.9320  3.6688  3.8910
    4.9995  3.0146  4.1015  4.5720
    5.9991  2.7705  4.0640  4.7890
    6.9985  2.2261  3.4699  4.3042
    7.9978  1.4402  2.3421  3.0200
    8.9969  0.4981  0.8278  1.0897
    698.0262 698.0852 698.0370 698.0283
    698.1548 698.1728 698.1563 698.1549
```

```
204           ,ratio,nSubP,'EdgyInt',EdgyInt,'hetCoeffs',cHetr);
205 patches.nu=0;
```

Form the Jacobian matrix, 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.

```
215     u0=0*patches.x; u0([1 end],:)=nan; u0=u0(:);
216     i=find(~isnan(u0));
217     nJ=length(i);
218     Jac=nan(nJ);
219     for j=1:nJ
220         u0(i)=((1:nJ)==j);
221         dudt=patchSys1(0,u0);
222         Jac(:,j)=dudt(i);
223     end
224     nonSkewSymmetric=norm(Jac+Jac')
225     assert(nonSkewSymmetric<1e-10,'failed skew-symmetry')
226     Jac(abs(Jac)<1e-12)=0;
```

Find the eigenvalues of the Jacobian, and list for inspection in [Table 3.3](#): the spectral interpolation is effectively exact for the macroscale; quadratic interpolation is usually qualitatively good; quartic interpolation appears to

be the lowest order for quantitative accuracy.

```

268 [evecs,evals]=eig(Jac);
269 maxRealPartEvals=max(abs(real(diag(evals))))
270 assert(maxRealPartEvals<1e-10,'failed real-part zero')
271 freqs=imag(diag(evals));

```

Use a count of zero crossings in the corresponding eigenvector in order to try to sort on the spatial wavenumber.

```

279 [~,j]=sort(sum(abs(diff(sign(real(evecs))))));
280 leadingFreqs=[leadingFreqs -freqs(j(1:2:nPatch+4))];

```

End of the for-loop over orders of interpolation, and display the spectra.

```

287 end
288 disp('      spectral      quadratic      quartic   sixth-order ...')
289 leadingFreqs = leadingFreqs

```

End of the main script.

3.9.2 waveFirst(): first-order wave PDE

This function codes a lattice, first-order, heterogeneous, wave PDE inside patches. Optionally adds some viscous dissipation. For 2D input arrays u and x (via edge-value interpolation of `patchSys1`, [Section 3.2](#)), computes the time derivative [\(3.6\)](#) at each point in the interior of a patch, output in ut .

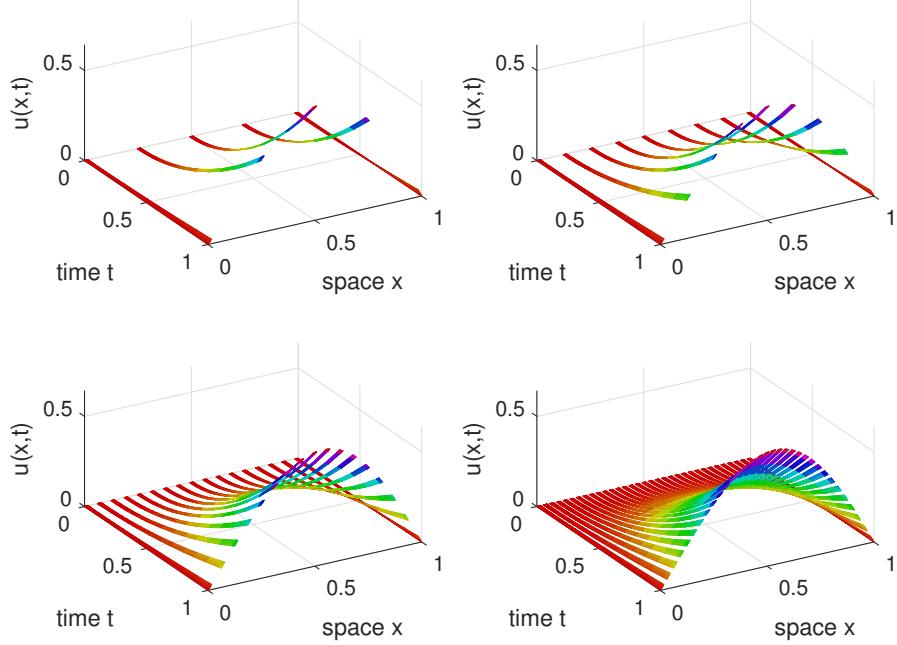
```

17 function ut = waveFirst(t,u,patches)
18     u=squeeze(u);
19     dx = diff(patches.x(2:3)); % space step
20     i = 2:size(u,1)-1; % interior points in a patch
21     ut = nan+u;          % preallocate output array
22     ut(i,:) = -(patches.cs(i).*u(i+1,:)) ...
23                 -patches.cs(i-1).*u(i-1,:))/(2*dx) ...
24                 +patches.nu*diff(u,2)/dx^2;
25 end% function

```

Fin.

Figure 3.16: diffusion field $u(x, t)$ of the patch scheme applied to the forced heterogeneous diffusive (3.7). Simulate for 5, 9, 17, 33 patches and compare to the full-domain simulation (65 patches, not shown).



3.10 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 & 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

$$\frac{\partial u_i}{\partial t} = \frac{1}{dx^2} \delta[a_{i-1/2} \delta u_i] + f_i(t), \quad (3.7)$$

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 3.16](#). 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 & Verfürth \(2022\)](#) reported much larger errors in the range 0.001–0.1 (Figure 3).

3.10.1 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.

```

78 clear all
79 %global OurCf2eps, OurCf2eps=true %option to save plots
80 mPeriod = 6
81 y = linspace(0,1,mPeriod+1)';
82 a = 1./(2-cos(2*pi*y(1:mPeriod)))
83 global microTimePeriod; microTimePeriod=0;

```

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

```

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

```

Loop to explore errors on various sized patches.

```

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

```

Determine indices of patches that are common in various resolutions

```

112 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 (3.7) solved on domain [0, 1], with `nP` patches, and say fourth order interpolation to provide the edge-values. Setting `patches.EdgeyInt` true means the edge-values come from interpolating the opposite next-to-edge values of the patches (not the mid-patch values).

```

127     global patches
128     ordCC = 4
129     configPatches1(@heteroDiffF,[0 1], 'equispace',nP ...
130                 ,ordCC,dx,nSubP,'EdgeyInt',true,'hetCoeffs',a);
131     DX = mean(diff(squeeze(patches.x(1,1,1,:))));
132     DXs=[DXs;DX];

```

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

```

140      if 0 % given forcing is exact
141          patches.f1=2*( patches.x-patches.x.^2 );
142          patches.f2=2*0.5+0*patches.x;
143      else% simple exp.sine forcing
144          patches.f1=sin(pi*patches.x).*exp(patches.x);
145          patches.f2=pi/2*sin(pi*patches.x).*exp(patches.x);
146      end%if

```

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

```

157      u0 = 0*patches.x;
158      tic
159      [ts,us] = ode15s(@patchSys1, [0 1], u0(:));
160      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.

```

173      xs = squeeze(patches.x);
174      us = patchEdgeInt1( permute( reshape(us ...
175          ,length(ts),nSubP,1,nP) ,[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));

```

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

```

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

```

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

```

203      i=nPeriodsPatch/2*mPeriod+1+(-mPeriod/2+1:mPeriod/2);
204      Us(:,:,iPP)=squeeze(us(i,end,I));
205      Xs=squeeze(patches.x(i,1,1,I));
206      if iPP>1
207          assert(norm(Xs-Xsp)<tol,'sampling error in space')
208          end

```

```

209      Xsp=Xs;
210  end%for log2Nx
211  ifOurCf2eps(mfilename) %optionally save plot
    Assess errors by comparing to the full-domain solution
217  DXs=DXs
218  Uerr=squeeze(max(max(abs(Us-Us(:,:,end))))) )
219  figure(2),clf,
220  loglog(DXs,Uerr,'o:')
221  xlabel('$H$'),ylabel('error')
222  ifOurCf2eps([mfilename 'Errs']) %optionally save plot

```

3.10.2 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.

```
17  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.

```

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

```

Two basic parameters, and initialise result array to NaNs.

```

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

```

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

```

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

```

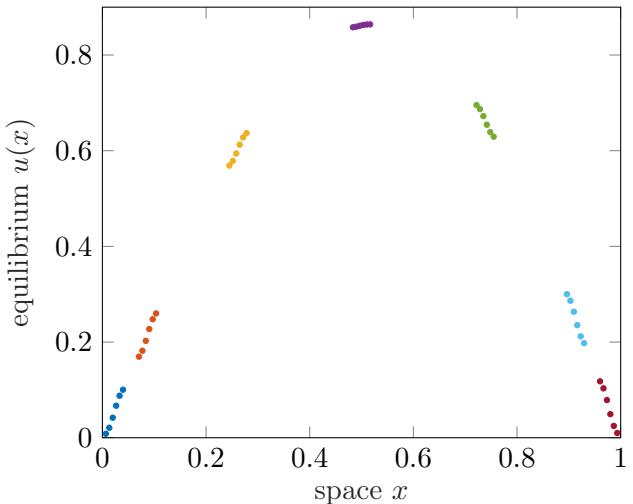
Code the microscale forced diffusion.

```

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

```

Figure 3.17: 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.



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

Sections 3.10 and 3.10.2 describe details of the problem and more details of the following configuration. The aim is to find the equilibrium, Figure 3.17, 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 3.17.

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

```

46 clear all
47 global patches
48 %global OurCf2eps, OurCf2eps=true %option to save plots
49 mPeriod = 6
50 y = linspace(0,1,mPeriod+1)';
51 a = 1./(2-cos(2*pi*y(1:mPeriod)))
52 global microTimePeriod; microTimePeriod=0;
```

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

```

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

Establish the global data struct `patches` for the microscale heterogeneous lattice diffusion system (3.7) solved on domain $[0, 1]$, with Chebyshev-like distribution of patches, and say fourth order interpolation to provide the

edge-values. Use ‘edgy’ interpolation.

```
77 ordCC = 4
78 configPatches1(@heteroDiffF,[0 1], 'chebyshev', nPatch ...
79 ,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.

```
88 if 0 % given forcing
89 patches.f1 = 2*( patches.x-patches.x.^2 );
90 patches.f2 = 2*0.5+0*patches.x;
91 else% simple exp-sine forcing
92 patches.f1 = sin(pi*patches.x).*exp(patches.x);
93 patches.f2 = pi/2*sin(pi*patches.x).*exp(patches.x);
94 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.

```
107 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.

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

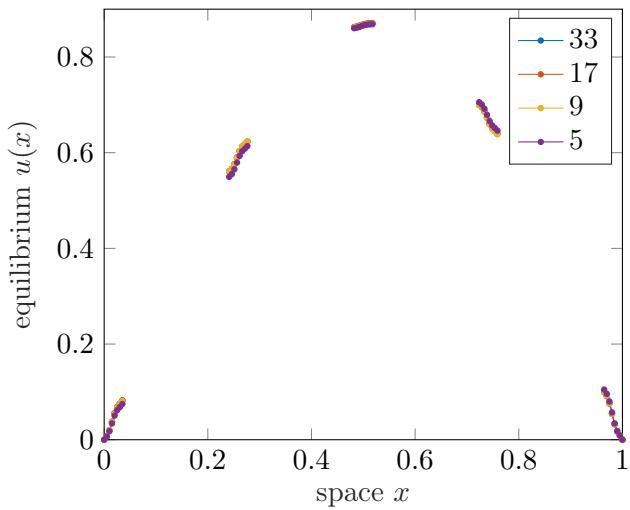
Seek the equilibrium, and report the norm of the residual, via the generic patch system wrapper `theRes` ([Section 3.19](#)).

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

Plot the equilibrium see [Figure 3.17](#).

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

Figure 3.18: 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.



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

Section 3.11 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 3.18 and 3.19. Find mean-abs errors to be the following:

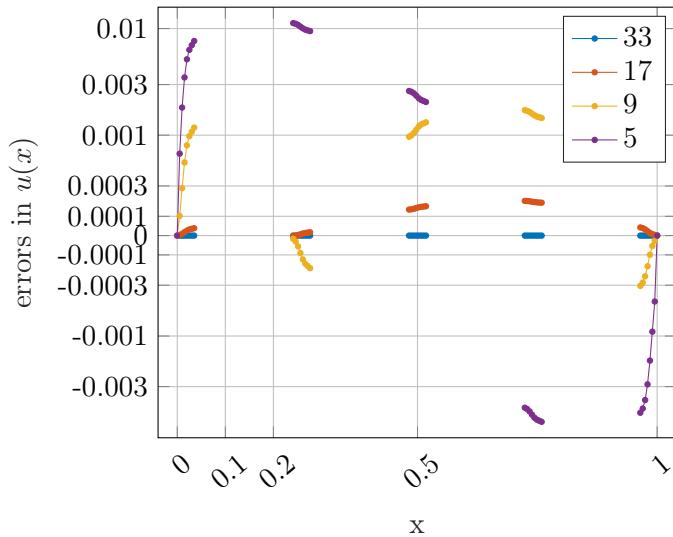
	$N =$	5	9	17	33	65
equispace	second-order	8E-3	1E-2	1E-2	4E-3	9E-4
equispace	fourth-order	2E-3	7E-4	1E-4	9E-6	5E-7
equispace	sixth-order	2E-3	2E-5	4E-7	1E-8	2E-10
chebyshev	second-order	4E-2	6E-2	3E-2	2E-2	2E-2
chebyshev	fourth-order	9E-4	3E-3	6E-4	3E-4	2E-4
chebyshev	sixth-order	9E-4	3E-5	1E-5	4E-6	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’¹¹. 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

¹¹ But the error assessment is with respect to finest patch-grid, no longer with a full domain solution

Figure 3.19: 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.



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).

```

136 clear all
137 global patches
138 %global OurCf2eps, OurCf2eps=true %option to save plots
139 switch 1
140     case 1, Dom.type = 'equispace'
141     case 2, Dom.type = 'chebyshev'
142     case 3, Dom.type = 'usergiven'
143 end% switch
144 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.

```

155 mPeriod = 6
156 z = (0.5:mPeriod)'/mPeriod;
157 a = 1./(2-cos(2*pi*z))
158 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 $\log 2N_{\max} = 129$ ($\epsilon = 0.008$) in a few seconds:

```

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

Set the periodicity  $\epsilon$ , and other microscale parameters.

177 nPeriodsPatch = 1 % any integer
178 nSubP = nPeriodsPatch*mPeriod+2 % for edgy int
179 epsilon = 1/(nPatchMax*nPeriodsPatch+1/mPeriod)
180 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.

```

193 us=[]; xs=[]; nPs=[]
194 for log2N=log2Nmax:-1:2
195     if log2N==log2Nmax
196         Ps=linspace(1,nPatchMax ...
197             ,5-2*all(Dom.type=='chebyshev'))
198     else Ps=(Ps+1)/2
199     end

```

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

```
205 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).

```

216 if all(Dom.type=='usergiven')
217     halfWidth=dx*(nSubP-1)/2;
218     X1 = 0+halfWidth; X2 = 1-halfWidth;
219     Dom.X = (X1+X2)/2-(X2-X1)/2*cos(linspace(0,pi,nPatch));
220 end

```

Configure the patches:

```

226 configPatches1(@heteroDiffF,[0 1],Dom,nPatch ...
227     ,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.

```

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

```

```

241     patches.f2 = pi/2*sin(pi*patches.x).*exp(patches.x);
242 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.

```

254 if log2N==log2Nmax
255 u0 = zeros(nSubP,1,1,nPatch);
256 else u0 = u0(:, :, :, 1:2:end);
257 end
258 u0([1 end], :) = nan;
259 patches.i = find(~isnan(u0));
260 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 3.19](#)).

```

269 tic;
270 [uSoln,resSoln] = fsolve(@theRes,u0(patches.i) ...
271 ,optimoptions('fsolve','Display','off'));
272 fsolveTime = toc

```

Store the solution into the `patches`, and give magnitudes— Inf norm is $\max(\text{abs}())$.

```

279 normSoln = norm(uSoln,Inf)
280 normResidual = norm(resSoln,Inf)
281 u0(patches.i) = uSoln;
282 u0 = patchEdgeInt1(u0);
283 u0( 1 , :, :, 1 ) = 0;
284 u0(end,:,:,:end) = 0;

```

Concatenate the solution on common patches into stores.

```

290 us=cat(3,us,squeeze(u0(:,:,:,Ps)));
291 xs=cat(3,xs,squeeze(patches.x(:,:,:,Ps)));
292 nPs = [nP;nP];

```

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

```

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

```

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

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

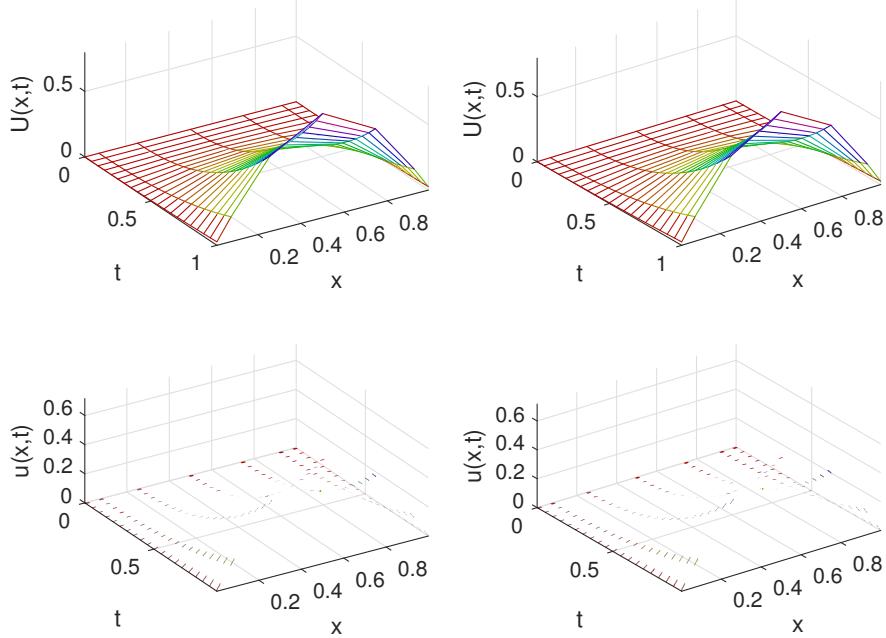
    Reshape solution field.

322 figure(1),clf
323 plot(x(:,u,'.-'), legend(num2str(nPs))
324 xlabel('space $x$'), ylabel('equilibrium $u(x)$')
325 ifOuRcf2tex([mfilename 'us'])%optionally save
```

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

```
333 err = u(:,1)-u;
334 figure(2), clf
335 h=plot(x(:,err,'.-'); legend(num2str(nPs))
336 quasiLogAxes(h,10,sqrt(prod(meanAbsErrs(2:3))))
337 xlabel('space $x$'), ylabel('errors in $u(x)$')
338 ifOuRcf2tex(mfilename)%optionally save
```

Figure 3.20: diffusion field $u(x, t)$ of the patch scheme applied to the forced space-time heterogeneous diffusive (3.8). 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.



3.13 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 & 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

$$\frac{\partial u_i}{\partial t} = \frac{1}{dx^2} \delta[a_{i+1/2}(t) \delta u_i] + f_i(t), \quad (3.8)$$

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 3.20](#) 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 only on a fraction of the spatial domain. Projective integration computes only on a fraction of the time domain determined by the ‘burst length’.

3.13.1 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.

```

98 clear all
99 %global OurCf2eps, OurCf2eps=true %option to save plots
100 mPeriod = 6
101 y = linspace(0,1,mPeriod+1)';
102 a = ( 3+cos(2*pi*y(1:mPeriod)) )/30
103 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.

```

116 nPeriodsPatch = 2 % any integer
117 rEpsilon = 100
118 dx = 1/(mPeriod*rEpsilon+1)
119 nSubP = nPeriodsPatch*mPeriod+2
120 tol=1e-9;

```

Set the time periodicity (global).

```

126 global microTimePeriod
127 microTimePeriod = 1/rEpsilon^2

```

Establish the global data struct `patches` for the microscale heterogeneous lattice diffusion system (3.8) 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).

```

144 nPatch = 7
145 ordCC = 4

```

```

146 Dom = 'chebyshev'
147 global patches
148 configPatches1(@heteroDiffF,[0 1],Dom,nPatch ...
149 ,ordCC,dx,nSubP,'EdgyInt',true,'hetCoeffs',a);
150 DX = mean(diff(squeeze(patches.x(1,1,1,:))))
Set the forcing coefficients as the odd-periodic extensions, accounting for
roundoff error in f2.

158 if 0 % given forcing
159   patches.f1=2*( patches.x-patches.x.^2 );
160   patches.f2=2*0.5+0*patches.x;
161 else% simple sine forcing
162   patches.f1=sin(pi*patches.x);
163   patches.f2=pi/2*sin(pi*patches.x);
164 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.

```

175 u0 = 0*patches.x;
176 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.

```

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

```

Time the projective integration simulation.

```

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

```

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

```

216 xs=squeeze(patches.x);
217 Xs=mean(xs);
218 Us=squeeze(mean( reshape(us,length(ts),[],nPatch), 2,'omitnan'));

```

```

219 figure(1),clf
220 for k = 1:2, subplot(2,2,k)
221 mesh(ts,Xs(:,Us'))
222 ylabel('space $x$'), xlabel('time $t$'), zlabel('$U(x,t)$')
223 colormap(0.8*hsv), axis tight, view(62-4*k,45)
224 end

```

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

```

232 xs([1 end],:) = nan;
233 for k = 1:2, subplot(2,2,2+k)
234 surf(tss,xs(:,uss', 'EdgeColor','none')
235 ylabel('space $x$'), xlabel('time $t$'), zlabel('$u(x,t)$')
236 colormap(0.7*hsv), axis tight, view(62-4*k,45)
237 end
238 ifOrCf2eps(mfilename)

```

3.13.2 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).

```

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

```

3.14 homoLanLif1D: computational homogenisation of a 1D heterogeneous Landau–Lifshitz by simulation on small patches

The Landau–Lifshitz equation describes the precessional motion of magnetization \vec{M} in a solid (see *Landau–Lifshitz–Gilbert equation* in Wikipedia). In a medium with microscale heterogeneity $a(x)$, and with phenomenological damping parameter α , we explore the dynamics of $\vec{M}(x, t)$ governed by the nonlinear Landau–Lifshitz PDE (Leitenmaier & Runborg 2021, (1.1)) ¹²

$$\vec{M}_t = -\vec{M} \times \vec{H} - \alpha \vec{M} \times (\vec{M} \times \vec{H}), \quad \vec{H} := \vec{\nabla} \cdot (a \vec{\nabla} \vec{M}).$$

Note, for every x , $|\vec{M}(x, t)|$ is constant in time due to $\vec{M} \cdot \vec{M}_t = 0$ for every x, t . We normally set $|\vec{M}(x, 0)| = 1$.

[Figure 3.21](#) shows an example simulation in time generated by the patch scheme applied to the above Landau–Lifshitz PDE on the spatial domain $[0, 1]$ with domain boundary conditions of 1-periodicity. The inter-patch coupling is realised by interpolation of the patch's next-to-edge values to the patch opposite edges. Such coupling preserves symmetry in many systems (quartic interpolation appears to be the lowest order that generally gives good accuracy). With damping parameter $\alpha = 0.001$ then the largest few macroscale modes decay with rate roughly 0.1, and so are negligibly damped over a time of 0.1.

Suppose the spatial microscale lattice is at points x_i , with constant spacing dx . With dependent variables $\vec{M}_i(t)$, simulate the microscale lattice system

$$\vec{M}_{it} = -\vec{M}_i \times \vec{H}_i - \alpha \vec{M}_i \times (\vec{M}_i \times \vec{H}_i), \quad \vec{H}_i := \frac{1}{dx^2} \delta[a_{i-1/2} \delta \vec{M}_i],$$

in terms of the centred difference operator δ . The system has a microscale heterogeneity via the coefficients $a_{i+1/2}$ which we assume to have some given known periodicity (Leitenmaier & Runborg 2021, pp.6,27). [Figure 3.21](#) shows a patch simulation of this system: observe the effects of the heterogeneity within each patch.

Parameters There are two closely related examples (Leitenmaier & Runborg 2021, pp.6,27), that we distinguish here with parameter `ex5p1`: set to either zero or one. The Landau–Lifshitz dissipation parameter α should be small. If the initial conditions are smooth, then `ode15s` has no problems for $\alpha = 0.001$. ¹³

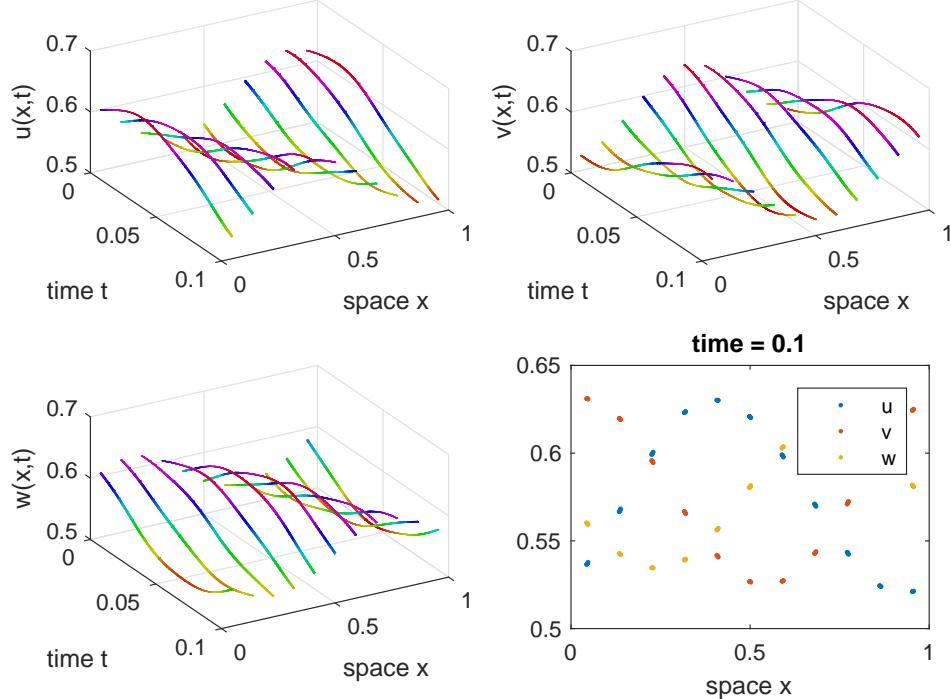
```
89 global alpha ex5p1
90 ex5p1 = 0; % set to 1 for L&O example of p.27
91 alpha = 0.001 % phenomenological damping parameter
```

The physical microscale periodicity of the heterogeneity is ϵ (ϵ is *not* the patch scale ratio):

¹² Recall $a \times (b \times c) = (a \cdot c)b - (a \cdot b)c$

¹³ But, add randomness to the initial conditions and the computation appears unstable with `ode15s` when $\alpha < 0.2$. However, `ode23` may be stable? for $\alpha = 0.01$ albeit expensively taking 10^7 time-steps per second (due to microscale oscillations of frequency up to 10^5 – 10^6).

Figure 3.21: magnetic field $\vec{M}(x, t) = (u, v, w)$ of the gap-tooth scheme applied to the heterogeneous Landau–Lifshitz PDE to show the emergent macroscale wave-like dynamics. This simulation uses eleven patches in space of size ratio 0.055. Compare the time $t = 0.1$ graph with Fig. 2.1 of Leitenmaier & Runborg (2021).



```
99 epsilon = 1/200/(1+ex5p1) %pp.6,27
```

3.14.1 Script code to simulate heterogeneous diffusion systems

This example script implements the following patch/gap-tooth scheme.

1. configPatches1
2. ode15s \mapsto patchSys1 \mapsto heteroLanLif1D
3. plot the simulation

First establish the microscale heterogeneity has micro-period `mPeriod` on the lattice with values of the column vector from Leitenmaier & Runborg (2021) [pp.6,27]. Later, the heterogeneity is repeated to fill each patch.

```
125 dx = 1/2000 %1/6000 %p.27
126 mPeriod = round(epsilon/dx)
127 a = 1 + 0.5*sin(2*pi*(0.5:mPeriod)'/mPeriod); %p.6
```

Establish the global data struct `patches` for the microscale heterogeneous lattice diffusion system (3.2) solved on 1-periodic domain, with maybe 24 patches, but 11 is enough, here each patch of size ratio to fit one period of the heterogeneity in each patch, and spectral inter-patch interpolation to provide the patch edge-values. Invoking `EdgyInt` means the edge-values come from interpolating the opposite next-to-edge values of the patches (not the mid-patch

values).

```

143 global patches
144 nPatch = 11 %24 %p.6, odd is slightly cleaner
145 nSubP = mPeriod+2
146 ratio = nPatch*epsilon
147 configPatches1(@heteroLanLif1D,[0 1],nan,nPatch ...
148     ,0,ratio,nSubP,'EdgyInt',true ...
149     ,'hetCoeffs',a);
150 assert(abs(dx-diff(patches.x(2:3)))<1e-10 ...
151     , 'microscale grid spacing error')
```

Simulate Set the initial conditions of a simulation to be that of [Leitenmaier & Runborg \(2021\)](#) [pp.6], except possibly perturbed by random microscale noise. Scale the initial conditions so that $|\vec{M}(x, 0)| = 1$.

```

163 u0 = 0.5+exp(-0.1*cos(2*pi*(patches.x-0.32)));
164 v0 = 0.5+exp(-0.2*cos(2*pi*patches.x)) +0*randn(size(patches.x));
165 w0 = 0.5+exp(-0.1*cos(2*pi*(patches.x-0.75)));
166 M0 = [ u0 v0 w0 ]./sqrt(u0.^2+v0.^2+w0.^2);
167 dM0dt = patchSys1(0,M0(:));
```

Integrate using standard integrators.

```

173 tic
174 [ts,Ms] = ode15s(@patchSys1, [0 0.1], M0(:));
175 cpuTime=toc
176 sizeMs=size(Ms)
```

Reshape results for processing. For simplicity, set edge values to `nans`. For the field values (which are rows in `Ms`) we need to reshape, permute, and reshape again.

```

185 xs = squeeze(patches.x);
186 Ms = reshape(Ms,length(ts),nSubP,3,nPatch);
187 Ms(:,[1 end],:,:) = nan; % nan patch edges
188 Ms = reshape(permute(Ms,[2 4 1 3]),[],length(ts),3);
```

Check on constancy of $|\vec{M}(x, t)|$ in time. The mean and standard deviation appears to show that, with `ode15s`, they are constant to errors typically 10^{-5} .

```

196 Mabs = sqrt( sum(Ms.^2,3) );
197 meanMabs = mean(Mabs(:),'omitnan')
198 stdevMabs = std(Mabs(:),'omitnan')
```

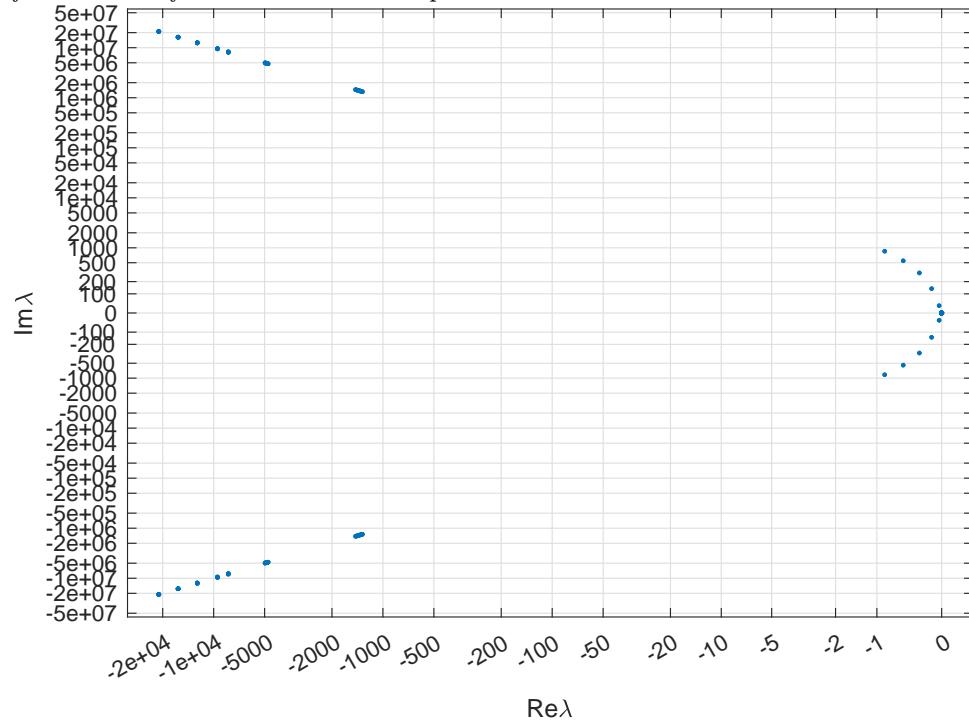
Plot space-time surface of the simulation Choose whether to save some plots, or not.

```

208 global OurCf2eps
209 OurCf2eps = false;
```

Subsampled surface over the macroscale duration of the simulation to show the propagation of the macroscale modes over the heterogeneous lattice.

Figure 3.22: spectrum of eigenvalues of the multiscale patch scheme applied to the Landau–Lifshitz PDE. The macroscale eigenvalues are clearly separated from those of the microscale sub-patch modes.



```

217 figure(1),clf
218 if length(ts)>50
219 [~,j]=min(abs(ts(:)-linspace(ts(1),ts(end),50)));
220 else j=1:length(ts); end
221 uvw='uvw';
222 for p=1:3
223 subplot(2,2,p)
224 mesh(ts(j),xs(:,Ms(:,j,p)))
225 view(60,40), colormap(0.8* hsv)
226 xlabel('time $t$'), ylabel('space $x$')
227 zlabel(['$', uvw(p) ,(x,t)$'])
228 end

```

Final time plot to compare with Fig. 2.1 of [Leitenmaier & Runborg \(2021\)](#).

```

235 subplot(2,2,4)
236 plot(xs(:,squeeze(Ms(:,end,:))),'.')
237 xlabel('space $x$'), legend(uvw(1),uvw(2),uvw(3))
238 title(['time = ' num2str(ts(end),4)])
239 if0urCf2eps([mfilename 'uvw'])

```

3.14.2 Spectrum of the coded patch system

It appears the spectrum has the following properties as shown by [Figure 3.22](#), with $N = \text{nPatch}$ and $n = \text{nSubP} - 2$, and on base of $\vec{M} = \vec{1}/\sqrt{3}$.

- A (near) zero eigenvalue for each and every microscale lattice point (nN) due to $|\vec{M}(x, t)|$ being constant in time, for every x . Presumably near zero (roughly 10^{-2}) due to round-off error.
- $2N$ macroscale eigenvalues, including a pair of (near) zero eigenvalues of macroscale conservation, and others ranging from $27(-\alpha \pm i)$ to $(-6.4\alpha \pm 7.4i)(N - 1)^2$.
- $2(n - 1)N$ fast eigenvalues, more negative than about $-\alpha \cdot 10^6$ and higher frequency than about 10^6 . Presumably depends upon ϵ —the periodicity and patch size.

Form an equilibrium of \vec{M} constant in space, then find the indices corresponding to patch interior points.

```

276 Me = 1+0.2*rand(1,3);
277 Me = Me./sqrt(sum(Me.^2,2))
278 Me = Me +0*patches.x;
279 Me([1 end],:,:, :)=nan;
280 i=find(~isnan(Me));
281 f0 = patchSys1(0,Me(:));
282 assert(abs( norm(f0(:)) )<1e-8,'not equilibrium')

```

Form the Jacobian by numerical differentiation.

```

288 delta=1e-7;
289 nJac=length(i);
290 Jac=nan(nJac);
291 for j=1:nJac
292     M=Me; M(i(j))=M(i(j))+delta;
293     fj=patchSys1(0,M(:));
294     Jac(:,j)=(fj(i)-f0(i))/delta;
295 end

```

Compute eigenvalues, sort, and count some groups according to ad hoc criteria.

```

302 eval = eig(Jac);
303 [~,k] = sort(abs(eval));
304 eval = eval(k);
305 nZero = sum(abs(eval)<1)
306 nCent = sum(abs(real(eval))<1e5*alpha)
307 nSlow = sum(abs(eval)<1e5)

```

Plot the spectrum of eigenvalues on quasi-log axes.

```

313 figure(2),clf
314 hp = plot(real(eval),imag(eval),'.');
315 xlabel('$\Re\lambda$'), ylabel('$\Im\lambda$')
316 quasiLogAxes(hp,1,100);
317 ifOurCf2eps([mfilename 'Spec'])

```

3.14.3 `heteroLanLif1D()`: heterogeneous Landau–Lifshitz PDE

This function codes the lattice heterogeneous Landau–Lifshitz PDE (Leitenmaier & Runborg 2021, (1.1)) inside patches in 1D space. For 4D input array M storing the three components of \vec{M} (via edge-value interpolation of `patchSys1`, Section 3.2), computes the time derivative at each point in the interior of a patch, output in Mt . The column vector of coefficients $c_i = 1 + \frac{1}{2} \sin(2\pi x_i/\epsilon)$ have previously been stored in struct `patches.cs`.

- With `ex5p1=0` computes the example EX1 (Leitenmaier & Runborg 2021, p.6).
- With `ex5p1=1` computes the first ‘locally periodic’ example (Leitenmaier & Runborg 2021, p.27).

```

29  function Mt = heteroLanLif1D(t,M,patches)
30      global alpha ex5p1
31      dx = diff(patches.x(2:3));    % space step

Compute the heterogeneous  $\vec{H} := \vec{\nabla} \cdot (a \vec{\nabla} \vec{M})$ 

37      a = patches.cs ...
38          +ex5p1*(0.1+0.25*sin(2*pi*(patches.x(2:end,:,:,:)-dx/2)+1.1));
39      H = diff(a.*diff(M))/dx^2;

```

At each microscale grid point, compute the cross-products $\vec{M} \times \vec{H}$ and $\vec{M} \times (\vec{M} \times \vec{H})$ to then give the time derivative $\vec{M}_t = -\vec{M} \times \vec{H} - \alpha \vec{M} \times (\vec{M} \times \vec{H})$ (Leitenmaier & Runborg 2021, (1.1)):

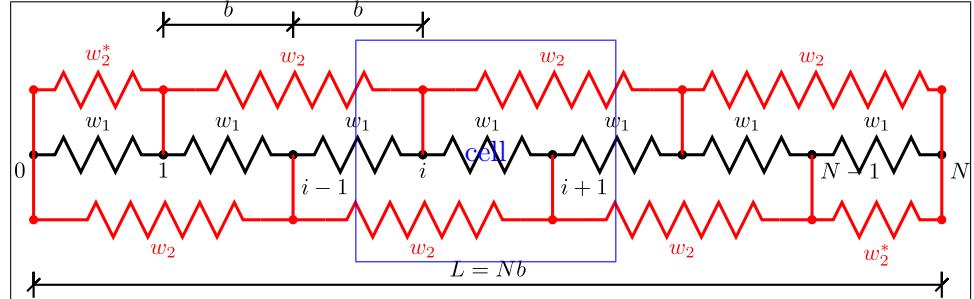
```

47      i = 2:size(M,1)-1;    % interior points in a patch
48      MH=nan+H; % preallocate for MxH
49      MH(:,3,:,:)=M(i,1,:,:).*H(:,2,:,:)-M(i,2,:,:).*H(:,1,:,:);
50      MH(:,2,:,:)=M(i,3,:,:).*H(:,1,:,:)-M(i,1,:,:).*H(:,3,:,:);
51      MH(:,1,:,:)=M(i,2,:,:).*H(:,3,:,:)-M(i,3,:,:).*H(:,2,:,:);
52      MMH=nan+H; % preallocate for MxMxH
53      MMH(:,3,:,:)=M(i,1,:,:).*MH(:,2,:,:)-M(i,2,:,:).*MH(:,1,:,:);
54      MMH(:,2,:,:)=M(i,3,:,:).*MH(:,1,:,:)-M(i,1,:,:).*MH(:,3,:,:);
55      MMH(:,1,:,:)=M(i,2,:,:).*MH(:,3,:,:)-M(i,3,:,:).*MH(:,2,:,:);
56      Mt = nan+M; % preallocate output array
57      Mt(i,:,:,:)= -MH-alpha*MMH;
58  end% function

```

Fin.

Figure 3.23: 1D arrangement of non-linear springs with connections to (a) next-to-neighbour node (Combescure 2022, Fig. 3(a)). The blue box is one micro-cell of one period, width $2b$, containing an odd and an even i .



3.15 Combescure2022: simulation and continuation of a 1D example nonlinear elasticity, via patches

Here we explore a nonlinear 1D elasticity problem with complicated microstructure. Executes a simulation. *But the main aim is to show how one may use the MatCont continuation toolbox (Govaerts et al. 2019) together with the Patch Scheme toolbox (Maclean et al. 2020) in order to explore parameter space by continuing branches of equilibria, etc.*

Figure 3.23 shows the microscale elasticity—adapted from Fig. 3(a) by Combescure (2022). Let the spatial microscale lattice be at rest at points x_i , with constant spacing b . 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 3.23) and for every i ,

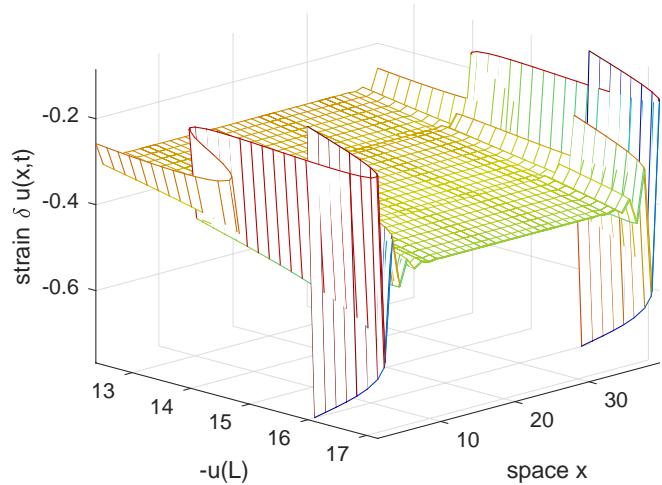
$$\begin{aligned} \epsilon_i^p &:= \frac{1}{pb}(u_{i+p/2} - u_{i-p/2}), & \sigma_i^p &:= w_p'(\epsilon_i^p), \\ \frac{\partial^2 u_i}{\partial t^2} &= \sum_{p=1}^2 \frac{1}{pb}(\sigma_{i+p/2}^p - \sigma_{i-p/2}^p), & w_p'(\epsilon) &:= \epsilon - M_p \epsilon^3 + \epsilon^5. \end{aligned} \quad (3.9)$$

The system has a microscale heterogeneity via the two different functions $w_p'(\epsilon)$ (Combescure 2022, §4):

- microscale ‘instability’ (structure) arises with $M_1 := 2$ and $M_2 := 1$ (Figures 3.24 and 3.27(b)); and
- large scale ‘instability’ (structure) arises with $M_1 := -1$ and $M_2 := 3$ (Figures 3.26 and 3.27(a)).

Microscale case Set $M_1 := 2$ and $M_2 := 1$. We fix the boundary conditions $u(0) = 0$ and parametrise solutions by $u(L)$. There are equilibria $u \approx u(L)x/L$, but under large compression (large negative $u(L)$) interesting structures develop. Figure 3.24 shows boundary layers with microscale variations develop for $u(L) < -13$. This figure plots a strain ϵ as the strain is nearly constant across the interior, so the boundary layers show up clearly. As $u(L)$ decreases further, Figure 3.24 shows the family of equilibria form complicated folds. Table 3.4 lists that MatCont also reports some branch

Figure 3.24: the case of microscale ‘instability’ appears as fluctuations close to both boundaries. As the system is physically compressed, the equilibrium curve has complicated folds, as shown here (and [Figure 3.27\(b\)](#)).



[Table 3.4:](#) Interesting equilibria for the cases of small scale instability: $M_1 := 2$, $M_2 := 1$ ([Figures 3.24](#) and [3.27\(b\)](#)). The rightmost column gives the $-u(L)$ parameter values for corresponding critical points in the three-patch code ([Figure 3.25](#)).

$-u(L)$	MatCont description	Patch
14.684	Branch point	14.599
14.702	Limit point	14.610
14.612	Neutral Saddle Equilibrium	-
14.063	Neutral Saddle Equilibrium	-
13.972	Limit point	13.817
13.988	Branch point	13.828
17.184	Branch point	17.197
-	Limit point	17.227
17.183	Neutral Saddle Equilibrium	17.211

points and neutral saddle equilibria in this same regime (see [Figure 3.27\(b\)](#)). I have not yet followed any of the branches.

The previous paragraph’s discussion is for a full domain simulation, albeit done through an imposed computational framework of physically abutting patches. [Figure 3.25](#) shows the corresponding MatCont continuation for the patch scheme with $N = 3$ patches in the domain. Just three patches may well be reasonable as the structures in this problem are the two boundary layers, and a constant interior. [Figure 3.25](#) shows the patch scheme reasonably resolves these. [Table 3.4](#) also lists the special points, as reported by MatCont, in the equilibria of the patch scheme. The locations of these special points reasonably match those found by the full domain simulation.

Importantly, MatCont is about *ten times quicker to execute on the patches* than on the full domain code. This speed-up indicates that on larger scale problems the patch scheme could be very useful in continuation explorations.

Large scale case Set $M_1 := -1$ and $M_2 := 3$. We fix the boundary conditions $u(0) = 0$ and parametrise solutions by $u(L)$. There are equilibria $u \approx u(L)x/L$, but under large compression (large negative $u(L)$) interesting structures develop. [Figure 3.26](#) shows an interior region of higher magnitude strain develops. Again, this figure plots a strain ϵ as the strain is nearly constant across the domain, so the interior structure shows up clearly. As $u(L)$

Figure 3.25: using just three patches, the case of microscale instability appears as fluctuations close to both boundaries. As the system is physically compressed, the equilibrium curve has complicated folds, as shown, and that approximately match [Figure 3.24](#). But it is computed ten times quicker.

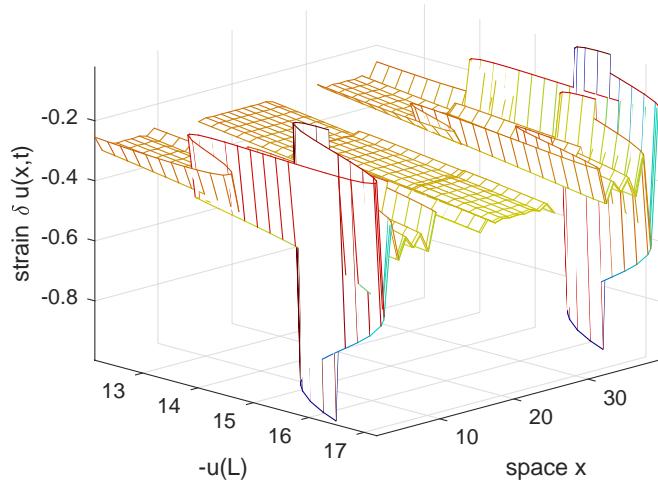
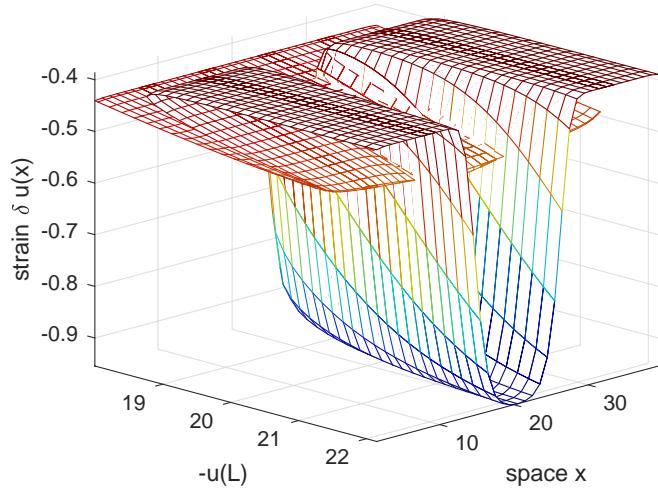


Figure 3.26: the case of large scale ‘instability’. Spatial structure appears in the middle of the domain. As the system is physically compressed, the equilibrium curve has complicated folds, as shown here and in [Figure 3.27\(a\)](#).



decreases further, [Figure 3.26](#) shows the family of equilibria form complicated folds. [Table 3.5](#) lists that MatCont also reports some branch points and neutral saddle equilibria in this regime (see [Figure 3.27\(a\)](#)). I have not yet followed any of the branches.

The patch scheme with $N = 3$ patches does not make reasonable predictions here. I suspect this failure is because the nontrivial interior structure here occupies too much of the domain to fit into one ‘small’ patch. Here the patch scheme may be useful if the physical domain is larger.

3.15.1 Configure heterogeneous toy elasticity systems

Set some physical parameters. Each cell is of width $dx := 2b$ as I choose to store u_i for odd i in $u((i+1)/2, 1, :)$ and for even i in $u(i/2, 2, :)$, that is,

	$-u(L)$	MatCont description
	21.295	Limit point
	18.783	Branch point
	18.762	Neutral Saddle Equilibrium
	18.761	Neutral Saddle Equilibrium
	18.761	Limit point
	18.934	Branch point
	19.393	Branch point
	19.928	Branch point
	20.490	Branch point
	21.055	Branch point
	21.627	Branch point

the physical displacements form the array

$$\mathbf{u} = \begin{bmatrix} u_1 & u_2 \\ u_3 & u_4 \\ u_5 & u_6 \\ \vdots & \vdots \end{bmatrix}.$$

Then corresponding velocities are adjoined as 3rd and 4th column.

```

229 clear all
230 global b M vis
231 b = 1 % separation of lattice points
232 N = 42 % # lattice steps in L
233 L = b*N % length of domain

```

The nonlinear coefficients of stress-strain are in array M , chosen by `theCase`.

```

240 theCase = 2
241 switch theCase
242 case 1, M = [0 0 0 0] % linear spring coefficients
243 case 2, M = [2 1 1 1] % micro scale instability??
244 case 3, M = [-1 3 1 1] % large scale instability??
245 end% switch
246 vis = 0.1 % does not appear to affect the equilibria
247 tEnd = 25

```

Patch parameters: here $nSubP$ is the number of cells.

```

253 edgyInt = true
254 nSubP = 6, nPatch = 5 % gives full-domain on N=42, dx=2
255 %nSubP = 6, nPatch = 3 % patches for some crude comparison

```

Establish the global data struct `patches` for the microscale heterogeneous lattice elasticity system (3.9). Solved with `nPatch` patches, and interpolation (as high-order as possible) to provide the edge-values of the inter-patch coupling conditions.

```

268 global patches
269 configPatches1(@heteroNLE,[0 L], 'equispace', nPatch ...

```

```

270      ,0,2*b,nSubP,'EdgyInt',edgyInt);
271  xx = patches.x+[-1 1]*b/2; % staggered sub-cell positions

```

3.15.2 Simulate in time

Set the initial displacement and velocity of a simulation. Integrate some time using standard integrator.

```

284 u0 = [ sin(pi/L*xx) -0*0.14*cos(pi/L*xx) ];
285 tic
286 [ts,ust] = ode23(@patchSys1, tEnd*linspace(0,1,41), u0(:) ...
287     ,[],patches,0);
288 cpuIntegrateTime = toc

```

Plot space-time surface of the simulation To see the edge values of the patches, interpolate and then adjoin a row of `nans` between patches. Because of the odd/even storage we need to do a lot of permuting and reshaping. First, array of sub-cell coordinates in a column for each patch, separating patches also by an extra row of nans.

```

301 xs = reshape( permute( xx ,[2 1 3 4]), 2*nSubP,nPatch);
302 xs(end+1,:) = nan;

```

Interpolate patch edge values, at all times simultaneously by including time data into the 2nd dimension, and 2nd reshaping it into the 3rd dimension.

```

310 uvs = reshape( permute( reshape(ust ...
311     ,length(ts),nSubP,4,1,nPatch) ,[2 3 1 4 5]) ,nSubP,[],1,nPatch);
312 uvs = reshape( patchEdgeInt1(uvs) ,nSubP,4,[],nPatch);

```

Extract displacement field, merge the 1st two columns, permute the time variations to the 3rd, separate patches by NaNs, and merge spatial data into the 1st column.

```

320 us = reshape( permute( uvs(:,1:2,:,:,:) ...
321     ,[2 1 4 3]) ,2*nSubP,nPatch,[]);
322 us(end+1,:,:,:) = nan;
323 us = reshape(us,[],length(ts));

```

Plot space-time surface of displacements over the macroscale duration of the simulation.

```

330 figure(1), clf()
331 mesh(ts,xs(:,),us)
332 view(60,40), colormap(0.8*jet), axis tight
333 xlabel('time $t$'), ylabel('space $x$'), zlabel('$u(x,t)$')

```

Ditto for the velocity.

```

339 vs = reshape( permute( uvs(:,3:4,:,:,:) ...
340     ,[2 1 4 3]) ,2*nSubP,nPatch,[]);
341 vs(end+1,:,:,:) = nan;
342 vs = reshape(vs,[],length(ts));
343 figure(2), clf()

```

```

344 mesh(ts, xs(:, ), vs)
345 view(60, 40), colormap(0.8*jet), axis tight
346 xlabel('time $t$'), ylabel('space $x$'), zlabel('$v(x,t)$')
347 drawnow

```

3.15.3 MatCont continuation

First, use `fsolve` to find an equilibrium at some starting compressive displacement—a compression that differs depending upon the case of nonlinearity.

```

359 muL0 = 12+6*(theCase==3)
360 u0 = [ -muL0*xx/L 0*xx ];
361 u0([1 end], :, :, :)=nan;
362 patches.i = find(~isnan(u0));
363 nVars=length(patches.i)
364 ueq=fsolve(@(v) dudtSys(0,v,muL0),u0(patches.i));

```

Start search for equilibria at other compression parameters. Starting from zero, need 1000+ to find both the large-scale and small-scale instability cases. But need less points when starting from parameter 12 or so.

```

373 disp('Searching for equilibria, may take 1000+ secs')
374 [uv0, vec0]=init_EP_EP(@matContSys, ueq, muL0, [1]);
375 opt=contset; % initialise MatCont options
376 opt=contset(opt, 'Singularities', true); %to report branch points, p.24
377 opt=contset(opt, 'MaxNumPoints', 400); % restricts how far matcont goes
378 opt=contset(opt, 'Backward', true); % strangely, needs to go backwards??
379 [uv, vec, s, h, f]=cont(@equilibrium, uv0, [], opt); %MatCont continuation

```

Post-process the report

```

386 disp('List of interesting critical points')
387 muLs=uv(nVars+1, :);
388 for j=1:numel(s)
389     disp([num2str(muLs(s(j).index), 5) ' & ' s(j).msg '\\"'])
390 end

```

Find a range of parameter and corresponding indices where all the critical points occur.

```

397 p1=muLs(end); pe=muLs(1);
398 if numel(s)>3, for j=2:numel(s)-1
399     p1=min(p1, muLs(s(j).index));
400     pe=max(pe, muLs(s(j).index));
401 end, end
402 pMid=(p1+pe)/2, pWid=abs(pe-p1)
403 iPars=find(abs(muLs(:)-pMid)<pWid); %include some either side

```

Choose an ‘evenly spaced’ subset of the range so we only plot up to sixty of the parameter values reported in the range.

```

411 nPars=numel(iPars)
412 dP=ceil((nPars-1)/60)

```

```
413 iP=1:dP:nPars;
414 muLP=muLs(iPars(iP));
```

Interpolate patch edge values, at all parameters simultaneously by including parameter-wise data into the 2nd dimension, and 2nd reshaping it into the 3rd dimension.

```
422 uvs=nan(numel(iP),numel(u0));
423 uvs(:,patches.i)=uv(1:nVars,iPars(iP))';
424 uvs = reshape( permute( reshape(uvs ...
425 ,length(muLP),nSubP,4,1,nPatch) ,[2 3 1 4 5]) ,nSubP,[],1,nPatch);
426 uvs = reshape( patchEdgeInt1(uvs) ,nSubP,4,[],nPatch);
```

Extract displacement field, merge the 1st two columns, permute the parameter variations to the 3rd, separate patches by NaNs, and merge spatial data into the 1st column.

```
434 us = reshape( permute( uvs(:,1:2,:,:,:) ...
435 ,[2 1 4 3]) ,2*nSubP,nPatch,[]);
436 us(end+1,:,:)= nan;
437 us = reshape(us,[],length(muLP));
```

Plot space-time surface of displacements over the macroscale duration of the simulation.

```
444 figure(4), clf()
445 mesh(muLP, xs(:,),us)
446 view(60,40), colormap(0.8*jet), axis tight
447 xlabel('-u(L)'), ylabel('space $x$'), zlabel('$u(x)$')
```

Plot space-time surface of strain, differences in displacements, over the parameter variation.

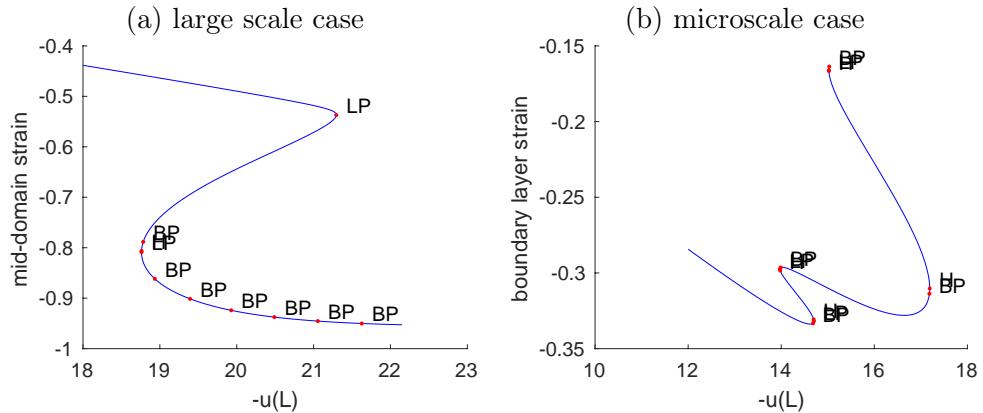
```
454 figure(5), clf()
455 mesh(muLP, xs(1:end-1),diff(us))
456 view(45,20), colormap(0.8*jet), axis tight
457 xlabel('$-u(L)$'), ylabel('space $x$'), zlabel('strain $\delta u(x)$')
458 ifOurCf2eps(['Comb22diffu' num2str(theCase)], [12 9])%optionally save
```

Labelled parameter plot Get the labelled 2D plots of [Figure 3.27](#) via MatCont's `cpl` function. In high-D problems it is unlikely that any one variable is a good thing to plot, so I show how to plot something else, here a strain. I use all the computed points so reform `uvs` (possibly better to have merged the critical points into the list of plotted parameters??).

```
488 uvs = nan(numel(muLs),numel(u0));
489 uvs(:,patches.i) = uv(1:nVars,:)';
490 uvs = reshape( uvs ,[],nSubP,4,nPatch);
```

As a function of the parameter, plot the strain in the middle of the domain (the middle of the middle patch), unless it is the microscale case when we plot a strain near the middle of the left boundary layer.

Figure 3.27: cross-sections through Figures 3.24 and 3.26: (a) large scale case, at the mid-point in space of Figure 3.26; (b) microscale case, in a boundary layer of Figure 3.24. These cross-sections are labelled with the various critical points.



```

499 if theCase==2, thePatch=1;
500 else thePatch=(nPatches+1)/2;
501 end%if
502 figure(7),clf
503 du = diff( uvs(:,nSubP/2,1:2,thePatch) ,1,3);
504 cpl([muLs;du'],[],s);
505 xlabel('$-u(L)$')
506 if thePatch==1, ylabel('boundary layer strain')
507 else ylabel('mid-domain strain')
508 end
509 if0urCf2eps(['Comb22cpl' num2str(theCase)], [9 7])%optionally save

```

3.15.4 matContSys: basic function for MatCont analysis

This is the simple ‘odefile’ of the patch scheme wrapped around the microcode.

```

522 function out = matContSys%(t,coordinates,flag,y,z)
523 out{1} = [];%@init;
524 out{2} = @dudtSys;
525 out{3} = [];%@jacobian;
526 out{4} = [];%@jacobianp;
527 out{5} = [];%@hessians;
528 out{6} = [];%@hessiansp;
529 out{7} = [];
530 out{8} = [];
531 out{9} = [];
532 end% function matContSys

```

3.15.5 dudtSys(): wraps around the patch wrapper

This function adjoins patches to the argument list, places the variables within the patch structure, and then extracts their time derivatives to return. Used

by both MatCont and `fsolve`.

```
545 function ut = dudtSys(t,u,p)
546 global patches
```

The 4 here is the number of variables in each micro-cell, that is, notionally ‘at’ each x -grid point.

```
553 U=nan(1,4)+patches.x;
554 U(patches.i)=u(:);
555 Ut=patchSys1(t,U,patches,p);
556 ut=Ut(patches.i);
557 end
```

3.15.6 `heteroNLE()`: forced heterogeneous elasticity

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

```
573 function uvt = heteroNLE(t,uv,patches,muL)
574 if nargin<4, muL=0; end% default end displacement is zero
575 global b M vis
```

Separate state vector into displacement and velocity fields: u_{ijI} is the displacement at the j th point in the i th 2-cell in the I th patch; similarly for velocity v_{ijI} . That is, physically neighbouring points have different j , whereas physical next-to-neighbours have i different by one.

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

Provide boundary conditions, here fixed displacement and velocity in the left/right sub-cells of the leftmost/rightmost patches.

```
595 u(1,:,:,:)=0;
596 v(1,:,:,:)=0;
597 u(end,:,:,:)=muL;
598 v(end,:,:,:)=0;
```

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

```
606 eps2 = diff(u)/(2*b);
607 eps1 = [u(:,2,:,:)-u(:,1,:,:) u([2:end 1],1,:,:)-u(:,2,:,:)]/b;
608 eps1(end,2,:,:)=nan; % as this value is fake
609 vx1 = [v(:,2,:,:)-v(:,1,:,:) v([2:end 1],1,:,:)-v(:,2,:,:)]/b;
610 vx1(end,2,:,:)=nan; % as this value is fake
```

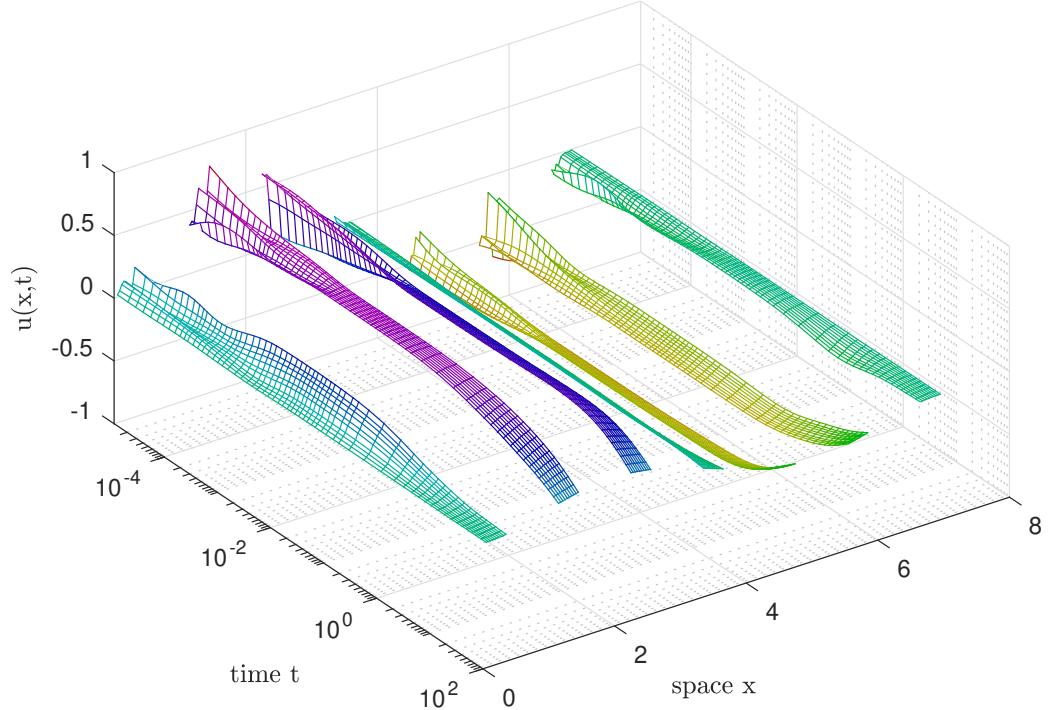
Set corresponding nonlinear stresses

```
616 sig2 = eps2-M(2)*eps2.^3+M(4)*eps2.^5;
617 sig1 = eps1-M(1)*eps1.^3+M(3)*eps1.^5;
```

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

```
625    uvt = nan+uv;           % preallocate output array
626    i=2:size(uv,1)-1;
627    % rate of change of position
628    uvt(i,1:2,:,:)= v(i,:,:,:);
629    % rate of change of velocity +some artificial viscosity??
630    uvt(i,3:4,:,:)= diff(sig2) ...
631        + [ sig1(i,1,:,:)-sig1(i-1,2,:,:)  diff(sig1(i,:,:,:),1,2)] ...
632        + vis*[ vx1(i,1,:,:)-vx1(i-1,2,:,:)  diff(vx1(i,:,:,:),1,2) ];
633
634 end% function heteroNLE
```

Figure 3.28: hyper-diffusing field $u(x, t)$ in the patch scheme applied to microscale heterogeneous hyper-diffusion (Section 3.16). The log-time axis shows: $t < 10^{-2}$, rapid decay of sub-patch micro-structure; $10^{-2} < t < 1$, meso-time quasi-equilibrium; and $1 < t < 10^2$, slow decay of macroscale structures.



3.16 hyperDiffHetero: simulate a heterogeneous hyper-diffusion PDE in 1D on patches

Section contents

3.16.1 Heterogeneous hyper-diffusion PDE inside patches . . . 136

Figure 3.28 shows an example simulation in time generated by the patch scheme applied to a heterogeneous version of the hyper-diffusion PDE. That such simulations makes valid predictions was established by Bunder et al. (2017) who proved that the scheme is accurate when the number of points in a patch is tied to a multiple of the periodicity of the pattern.

We aim to simulate the heterogeneous hyper-diffusion PDE

$$u_t = -D[c_1(x)Du] \quad \text{where operator } D := \partial_x(c_2(x)\partial_x), \quad (3.10)$$

for microscale periodic coefficients $c_l(x)$, and boundary conditions of $u = u_x = 0$ at $x = 0, L$. In this 1D space, the macroscale, homogenised, effective hyper-diffusion should be some unknown ‘average’ of these coefficients, but we use the patch scheme to provide a computational homogenisation. We discretise the PDE to a lattice of values $u_i(t)$, with lattice spacing dx , and

governed by

$$\dot{u}_i = -D[c_{i1}Du_i] \quad \text{where operator } D := \delta(c_{i2}\delta)/dx^2$$

in terms of centred difference operator $\delta u_i := u_{i+1/2} - u_{i-1/2}$.

Set the desired microscale periodicity, and correspondingly choose random microscale diffusion coefficients (with some subscripts shifted by a half).

```
57 clear all
58 basename = mfilename
59 %global OurCf2eps, OurCf2eps=true %optional to save plots
60 nGap = 3 % controls size of gap between patches
61 nPtsPeriod = 5
62 dx = 0.5/nGap/nPtsPeriod
```

Create some random heterogeneous coefficients, log-uniform.

```
69 csVar = 1
70 cs = 0.2*exp( -csVar/2+csVar.*rand(nPtsPeriod,2) )
```

Establish global data struct `patches` for heterogeneous hyper-diffusion on a finite domain with, on average, one patch per unit length. Use seven patches, and use high-order interpolation with `ordCC = 0`.

```
80 nPatch = 7
81 nSubP = 2*nPtsPeriod+4 % or +2 for not-edgyInt
82 Len = nPatch;
83 ordCC = 0;
84 dom.type = 'equispace';
85 dom.bcOffset = 0.5 % for BC type
86 patches = configPatches1(@hyperDiffPDE, [0 Len], dom ...
87 ,nPatch,ordCC,dx,nSubP,'EdgyInt',true,'nEdge',2 ...
88 , 'hetCoeffs',cs);
89 xs=squeeze(patches.x);
```

Simulate in time Set an initial condition, and here integrate forward in time using a standard method for stiff systems—because of the simplicity of linear problems this method works quite efficiently here. Integrate the interface `patchSys1` ([Section 3.2](#)) to the microscale differential equations.

```
103 u0 = sin(2*pi/Len*patches.x).*rand(nSubP,1,1,nPatch);
104 tic
105 [ts,us] = ode15s(@patchSys1, [0 100], u0(:),[],patches);
106 simulateTime = toc
107 us = reshape(us,length(ts),numel(patches.x(:))),[]);
```

Plot the simulation in [Figure 3.28](#), using log-axis for time so we can see a little of both micro- and macro-dynamics.

```
116 figure(1),clf
117 xs([1:2 end-1:end],:) = nan;
118 t0=min(find(ts>1e-5));
119 mesh(ts(t0:3:end),xs(:,us(t0:3:end,:))), view(55,50)
```

```

120 colormap(0.7*hsv)
121 xlabel('time $t$'), ylabel('space $x$'), zlabel('$u(x,t)$')
122 ca=gca; ca.XScale='log'; ca.XLim=ts([t0 end]);
123 ifOursCf2eps([basename 'Uxt'])

```

Fin.

3.16.1 Heterogeneous hyper-diffusion PDE inside patches

As a microscale discretisation of hyper-diffusion PDE (3.10) $u_t = -D[c_1(x)Du]$, where heterogeneous operator $D = \partial_x(c_2(x)\partial_x)$.

```

138 function ut=hyperDiffPDE(t,u,patches)
139 dx=diff(patches.x(1:2)); % microscale spacing

```

Code Dirichlet boundary conditions of zero function and derivative at left-end of left-patch, and right-end of right-patch. For slightly simpler coding, squeeze out the two singleton dimensions.

```

148 u = squeeze(u);
149 if ~patches.periodic % discretise BC u=u_x=0
150 u(1:2,1)=0;
151 u(end-1:end,end)=0;
152 end%if

```

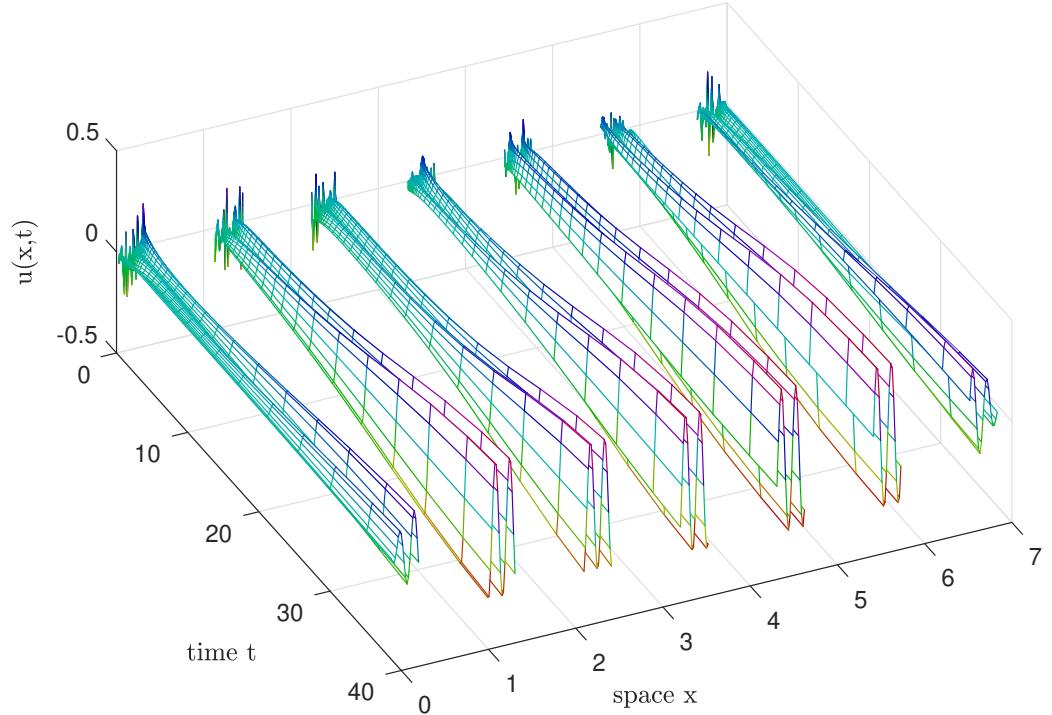
Here code straightforward centred discretisation in space.

```

158 ut = nan+u; % preallocate output array
159 v = patches.cs(2:end,1).*diff(patches.cs(:,2).*diff(u))/dx^2;
160 ut(3:end-2,:) = -diff(patches.cs(2:end-1,2).*diff(v))/dx^2 ;
161 end

```

Figure 3.29: the pattern forming field $u(x, t)$ in the patch (gap-tooth) scheme applied to a microscale discretisation of the Swift–Hohenberg PDE (Section 3.17). Physically we see the rapid decay of much microstructure, but also the meso-time growth of sub-patch-scale patterns, wavenumber k_0 , that are modulated over the inter-patch distances and over long times.



3.17 SwiftHohenbergPattern: patterns of the Swift–Hohenberg PDE in 1D on patches

Section contents

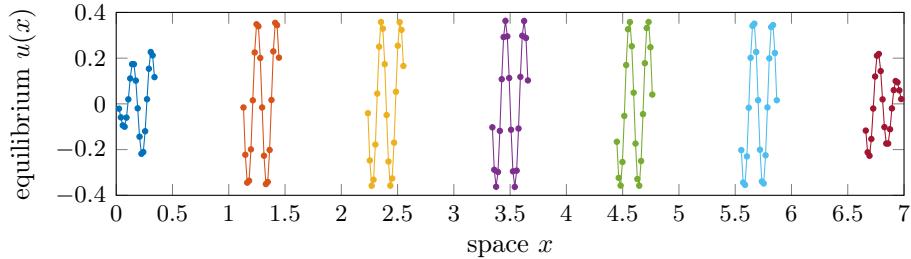
3.17.0.1 Find equilibrium with fsolve	138
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Figure 3.29 shows an example simulation in time generated by the patch scheme applied to the patterns arising from the Swift–Hohenberg PDE. That such simulations of patterns makes valid predictions was established by Bunder et al. (2017) who proved that the scheme is accurate when the number of points in a patch is just more than a multiple of the periodicity of the pattern.

Consider a lattice of values $u_i(t)$, with lattice spacing dx , and governed by a microscale centred discretisation of the Swift–Hohenberg PDE

$$\partial_t u = -(1 + \partial_x^2/k_0^2)^2 u + Ra u - u^3, \quad (3.11)$$

Figure 3.30: an equilibrium of the Swift–Hohenberg PDE on seven patches in 1D space. In the sub-patch patterns, there is a small phase shift in the patterns from patch to patch. And the amplitude of the pattern has to go to ‘zero’ at the boundaries.



with boundary conditions of $u = u_x = 0$ at $x = 0, L$. For Ra just above critical, say $\text{Ra} = 0.1$, the system rapidly evolves to spatial quasi-periodic solutions with period ≈ 0.166 when wavenumber parameter $k_0 = 38$. On medium times these spatial oscillations grow to near equilibrium amplitude of $\sqrt{\text{Ra}}$, and over very long times the phases of the oscillations evolve in space to adapt to the boundaries.

Set the desired microscale periodicity of the emergent pattern.

```

52 clear all, close all
53 %global OurCf2eps, OurCf2eps=true %optional to save plots
54 Ra = 0.1 % Ra>0 leads to patterns
55 nGap = 3
56 %waveLength = 0.496688741721854 /nGap %for nPatch==5
57 waveLength = 0.497630331753555 /nGap %for nPatch==7
58 %waveLength = 0.5 /nGap %for periodic case
59 nPtsPeriod = 10
60 dx = waveLength/nPtsPeriod
61 k0 = 2*pi/waveLength

```

Establish global data struct patches for the Swift–Hohenberg PDE on some length domain. Use seven patches. Quartic (fourth-order) interpolation $\text{ordCC} = 4$ provides values for the inter-patch coupling conditions.

```

72 nPatch = 7
73 nSubP = 2*nPtsPeriod+4
74 %nSubP = 2*nGap*nPtsPeriod+4 % full-domain
75 Len = nPatch;
76 ordCC = 4;
77 dom.type='equispace';
78 dom.bcOffset=0.5
79 patches = configPatches1(@SwiftHohenbergPDE,[0 Len],dom ...
80 ,nPatch,ordCC,dx,nSubP,'EdgyInt',true,'nEdge',2);
81 xs=squeeze(patches.x);

```

3.17.0.1 Find equilibrium with fsolve

Start the search from some guess.

```

103 fprintf('\n**** Find equilibrium with fsolve\n')
104 u = 0.4*sin(k0*patches.x);

```

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

```

112 u([1:2 end-1:end],:) = nan;
113 patches.i = find(~isnan(u));

```

Seek the equilibrium, and report the norm of the residual, via the generic patch system wrapper `theRes` ([Section 3.19](#)).

```

121 tic
122 [u(patches.i),res] = fsolve(@(v) theRes(v,patches,k0,Ra) ...
123     ,u(patches.i) ,optimoptions('fsolve','Display','off'));
124 solveTime = toc
125 normRes = norm(res)
126 assert(normRes<1e-6,'**** fsolve solution not accurate')

```

Plot the equilibrium see [Figure 3.30](#).

```

134 figure(1),clf
135 subplot(2,1,1)
136 plot(xs,squeeze(u),'.-')
137 xlabel('space $x$'),ylabel('equilibrium $u(x)$')
138 ifOurCf2tex([mfilename 'Equilib'])%optionally save

```

3.17.0.2 Simulate in time

Set an initial condition, and here integrate forward in time using a standard method for stiff systems—because of the simplicity of linear problems this method works quite efficiently here. Integrate the interface `patchSys1` ([Section 3.2](#)) to the microscale differential equations.

```

155 fprintf('\n**** Simulate in time\n')
156 u0 = 0*patches.x+0.1*randn(nSubP,1,1,nPatch);
157 tic
158 [ts,us] = ode15s(@patchSys1, [0 40], u0(:) ,[],patches,k0,Ra);
159 simulateTime = toc
160 us = reshape(us,length(ts),numel(patches.x(:)),[]);

```

Plot the simulation in [Figure 3.29](#).

```

167 figure(2),clf
168 xs([1:2 end-1:end],:) = nan;
169 mesh(ts(1:3:end),xs(:,us(1:3:end,:))), view(65,60)
170 colormap(0.7*hsv)
171 xlabel('time $t$'), ylabel('space $x$'), zlabel('$u(x,t)$')
172 ifOurCf2eps([mfilename 'Uxt'])

```

Fin.

3.17.1 The Swift–Hohenberg PDE and BCs inside patches

As a microscale discretisation of Swift–Hohenberg PDE $u_t = -(1 + \partial_x^2/k_0^2)^2 u + Ra u - u^3$, here code straightforward centred discretisation in space.

```
186 function ut=SwiftHohenbergPDE(t,u,patches,k0,Ra)
187     dx=diff(patches.x(1:2)); % microscale spacing
188     i=3:size(u,1)-2; % interior points in patches
```

Code Dirichlet boundary conditions of zero function and derivative, $u = u_x = 0$, at the left-end of the leftmost-patch, and the right-end of the rightmost-patch. For slightly simpler coding, squeeze out the two singleton dimensions.

```
198     u = squeeze(u);
199     u(1:2,1)=0;
200     u(end-1:end,end)=0;
```

Here code straightforward centred discretisation in space.

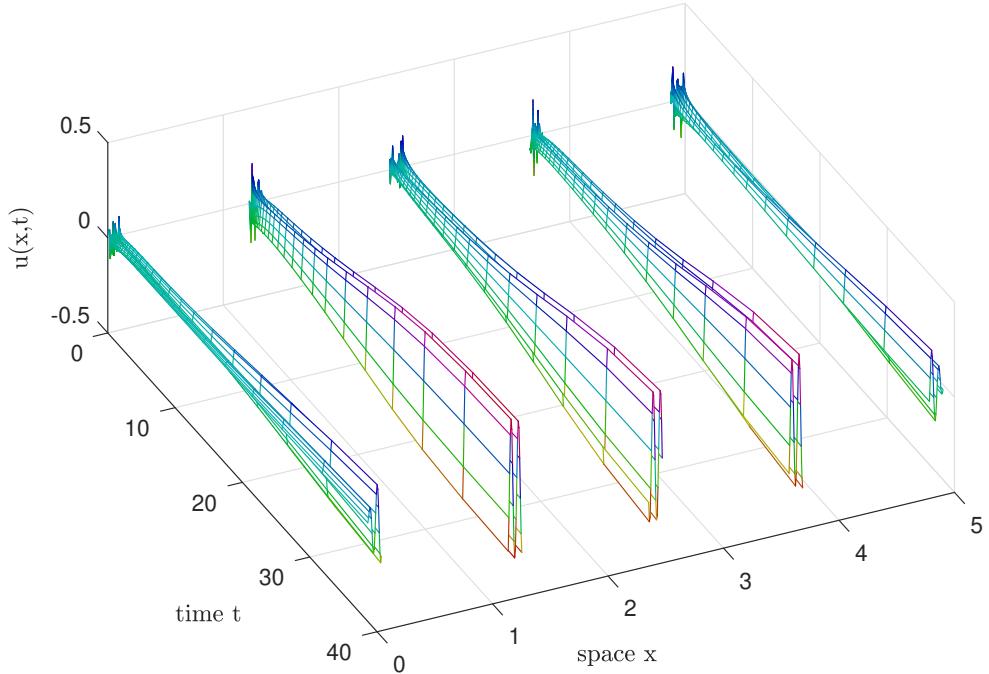
```
206     ut=nan+u;           % preallocate output array
207     v = u(2:end-1,:)+diff(u,2)/dx^2/k0^2;
208     ut(i,:) = - ( v(2:end-1,:)+diff(v,2)/dx^2/k0^2 ) ...
209         +Ra*u(i,:)-u(i,:).^3;
210 end
```

3.17.2 theRes(): wrapper function to zero for equilibria

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

```
225 function f=theRes(u,patches,k0,Ra)
226     v=nan(size(patches.x));
227     v(patches.i) = u;
228     f = patchSys1(0,v(:,),patches,k0,Ra);
229     f = f(patches.i);
230 end%function theRes
```

Figure 3.31: the field $u(x, t)$ in the patch (gap-tooth) scheme applied to microscale heterogeneous Swift–Hohenberg PDE (Section 3.18). The heterogeneous coefficients are approximately uniform over $[0.9, 1.1]$. This heterogeneity has no noticeable affect on the simulation.



3.18 SwiftHohenbergHetero: patterns of a heterogeneous Swift–Hohenberg PDE in 1D on patches

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Figure 3.31 shows an example simulation in time generated by the patch scheme applied to the patterns arising from a heterogeneous version of the Swift–Hohenberg PDE. That such simulations of patterns makes valid predictions was established by Bunder et al. (2017) who proved that the scheme is accurate when the number of points in a patch is tied to a multiple of the periodicity of the pattern.

Consider a lattice of values $u_i(t)$, with lattice spacing dx , arising from a microscale discretisation of the pattern forming, heterogeneous, Swift–Hohenberg PDE

$$\partial_t u = -D[c_1(x)Du] + Ra u - u^3, \quad D := 1 + \partial_x[c_2(x)\partial_x \cdot]/k_0^2, \quad (3.12)$$

where $c_\ell(x)$ have period $2\pi/k_0$. Coefficients c_ℓ are chosen iid random, nearly uniform, with mean near one. With mean one, the periodicity of c_ℓ approximately matches the periodicity of the resultant spatial pattern.

The current patch scheme coding preserves symmetry in the case of periodic patches (for every order of interpolation). For equispace and chebyshev options, the coupling currently fails symmetry.

Consider the spectrum in the symmetric cases of periodic patches (based upon only the cases $N = 5, 7$). There are $2N$ small eigenvalues, separated by a gap from the rest. In the homogeneous case, these occur as N pairs. With small heterogeneity, they appear to split into $N - 1$ pairs, and two distinct. With stronger heterogeneity (say 0.5), they *often* appear to also split into two clusters, each of N eigenvalues, with one small-valued cluster, and one meso-valued cluster—curious. Further analysis with sparse approximation of the invariant spaces suggests the following:

- for homogeneous, the $2N$ modes are local oscillations in each patch, with two modes each corresponding to phase shifts of the possible oscillations;
- for heterogeneous
 - N eigenmodes appear to be one phase ‘locking’ to the heterogeneity; and
 - N eigenmodes appear to be other phase ‘locking’ to the heterogeneity. Unless it is something to do with the coupling, but then it only appears with heterogeneity.

Consider the spectrum with BCs of $u = u_{xx} = 0$ at ends. Non-symmetric so some eigenvalues are complex! For small or zero heterogeneity find $2N - 2$ eigenvalues are small. Effectively, two modes in each of $N - 2$ interior patches, and one mode each in the two end patches. With increasing heterogeneity (say above 0.3), the gap decreases as a couple (or some) of the small eigenvalues become larger in magnitude.

Consider the spectrum with BCs of $u = u_x = 0$ at ends. Non-symmetric so some eigenvalues are complex! For small or zero heterogeneity find $2N - 4$ eigenvalues are small. Effectively, two modes in each of $N - 2$ interior patches. With increasing heterogeneity (say above 0.4), half ($N - 2$) of the small eigenvalues become larger in magnitude (presumably some phase ‘locking’ to the heterogeneity): effectively forms two clusters of modes.

Set the desired microscale periodicity of the patterns, here 0.062, and on the microscale lattice of spacing 0.0062, correspondingly choose random microscale material coefficients. The wavenumber of this microscale patterns is $k_0 \approx 101$.

```

102 clear all
103 %global OurCf2eps, OurCf2eps=true %optional to save plots
104 basename = ['r' num2str(floor(1e5*rem(now,1))) mfilename]
105 Ra = 0.1 % Ra>0 leads to patterns
106 nGap = 8 % controls size of gap between patches

```

```

107 waveLength = 0.496688741721854 /nGap %for nPatch==5
108 %waveLength = 0.497630331753555 /nGap %for nPatch==7
109 %waveLength = 0.5 /nGap %for periodic case
110 nPtsPeriod = 10
111 dx = waveLength/nPtsPeriod
112 k0 = 2*pi/waveLength

```

Create some random heterogeneous coefficients.

```

119 heteroVar = 0.99*[1 1] % must be <2
120 c1 = 1./(1-heteroVar/2+heteroVar.*rand(nPtsPeriod,2));
121 cRange = quantile(c1,0:0.5:1)

```

Establish global data struct `patches` for heterogeneous Swift–Hohenberg PDE with, on average, one patch per units length. Use seven patches to start with. Quartic (fourth-order) interpolation `ordCC = 4` provides values for the inter-patch coupling conditions. Or use as high-order as possible with `ordCC = 0`.

```

133 nPatch = 5
134 nSubP = 2*nPtsPeriod+4 % +2 for not-edgyInt
135 %nSubP = 2*nGap*nPtsPeriod+4 % approx full-domain
136 Len = nPatch;
137 ordCC = 0;
138 dom.type='equispace';
139 dom.bcOffset=0.5
140 patches = configPatches1(@heteroSwiftHohenbergPDE,[0 Len],dom ...
141 ,nPatch,ordCC,dx,nSubP,'EdgyInt',true,'nEdge',2 ...
142 , 'hetCoeffs',c1);
143 xs=squeeze(patches.x);

```

3.18.0.1 Explore the Jacobian

Finds that with periodic patches, everything is symmetric. However, for equispace or chebyshev, the patch coupling is not symmetric—is this to be expected?

```

155 fprintf('\n**** Explore the Jacobian\n')
156 u0 = 0*patches.x;
157 u0([1:2 end-1:end],:) = nan;
158 patches.i = find(~isnan(u0));
159 nVars = numel(patches.i)
160 Jac = nan(nVars);
161 for j=1:nVars
162     Jac(:,j)=theRes((1:nVars)==j,patches,k0,0,0);
163 end

```

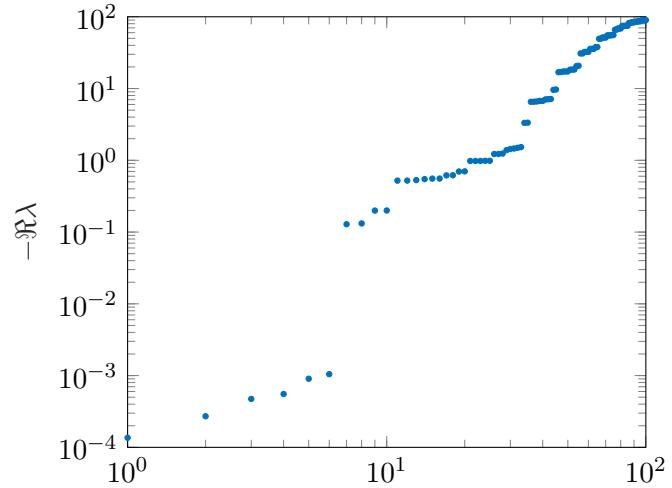
Check on the symmetry of the Jacobian

```

169 nonSymmetric = norm(Jac-Jac')
170 Jac(abs(Jac)<1e-12)=0;
171 antiJac = Jac-Jac';

```

Figure 3.32:
 eigenvalues of the patch scheme on the heterogeneous Swift–Hohenberg PDE (linearised). With $N = 5$ patches and BCS of $u = u_x = 0$ at $x \in \{0, 5\}$, there are $2(N - 2) = 6$ small eigenvalues, $|\lambda| < 0.001$, corresponding to six slow modes in the interior.



```

172 antiJac(abs(antiJac)<1e-12)=0;
173 figure(6),clf
174 spy(Jac,'.'),hold on, spy(antiJac,'rx'),hold off
175 if nonSymmetric>5e-9, warning('failed symmetry'),
176 else Jac = (Jac+Jac')/2; %tweak to symmetry
177 end

```

Compute eigenvalues and eigenvectors.

```

183 figure(5),clf
184 [levec,mEval] = eig(-Jac , 'vector');
185 [~,j]=sort(real(mEval));
186 mEval=mEval(j); evec=levec(:,j);
187 loglog(real(mEval),'.')
188 ylabel('$-\text{Re}\lambda$')
189 ifOurCf2tex([basename 'Eval'])%optionally save

```

Explore sparse approximations of all the slowest together (lots of iterations required), or separately of the two clusters of the slowest (few iterations needed). First ascertain whether one or two clusters of small eigenvalues.

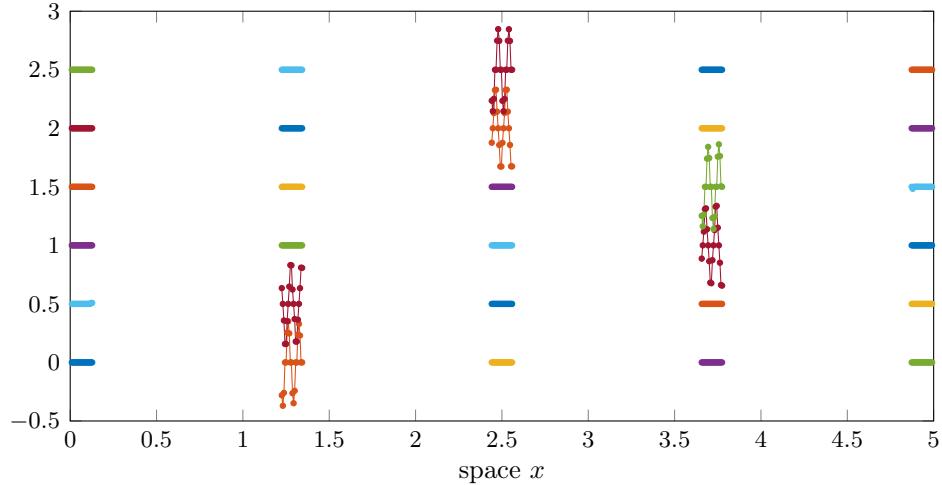
```

210 logGaps=diff(log10(real(mEval)));
211 [~,j]=sort(-logGaps);
212 %someLogGaps=[logGaps(j(1:5)) j(1:5)]
213 if logGaps(j(2))<0.4*logGaps(j(1)), nSlow=j(1)
214 else nSlow=min( sort(j(1:2)) , 3*nPatch)
215 end
216 log10Gap=logGaps(nSlow)
217 smallEvals=-mEval(1:nSlow(end)+2)

```

Second, make eigenvectors all real, sparsely approximate cluster modes via an algorithm developed from [Hu et al. \(2016\)](#), and plot. [Figure 3.33](#) shows that each pair of basis vectors are phase-shifted by 90° .

Figure 3.33: sparse approximations of the eigenvectors of the six slow modes of Figure 3.32. Plotted are sparse basis vectors for the invariant space spanned by the six slow eigenvectors: each basis vector shifted vertically to separate. Thus a fair approximation is that there are effectively two modes for each of the $N - 2 = 3$ interior patches.



```

227 js=find(imag(mEval)>0);
228 evec(:,js)=imag(evec(:,js));
229 evec=real(evec);
230 if numel(nSlow)==1, S = spcart(evec(:,1:nSlow));
231 else S = spcart(evec(:,1:nSlow(1)));
232 S = [S spcart(evec(:,nSlow(1)+1:nSlow(2)) ] ;
233 end;
234 figure(3),clf
235 vStep=ceil(max(abs(S(:)))*10+1)/10
236 for j=1:nSlow(end)
237 u0(patches.i)=S(:,j);
238 plot(xs,vStep*(j-1)+squeeze(u0),'.-'),hold on
239 end
240 hold off, xlabel('space $x$')
241 ifOurCf2tex([basename 'Evec'])%optionally save

```

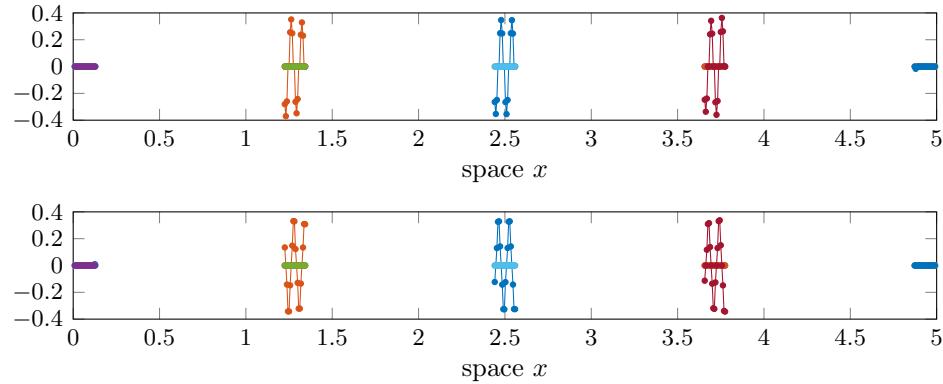
Reorganise the eigenvectors to maybe clarify.

```

262 [i,j]=find(abs(S)>vStep/2);
263 j=find([1;diff(j)]);
264 [i,k]=sort(i(j));
265 figure(4)
266 for p=1:2
267 clf, subplot(2,1,1)
268 for j=p:2:numel(k)
269 u0(patches.i)=S(:,k(j));
270 plot(xs,squeeze(u0),'.-'),hold on
271 end% for j
272 hold off, xlabel('space $x$')

```

Figure 3.34: sparse basis approximations for the invariant subspace of the six slow modes of Figure 3.32. A replot of Figure 3.33 but with three of the basis vectors superimposed in each of the two panels.



```

273     ifOurCf2tex([basename 'Evec' num2str(p)])%optionally save
274 end%for p

```

3.18.0.2 Find an equilibrium with fsolve

Start the search from some guess.

```

297 fprintf('\n**** Find equilibrium with fsolve\n')
298 u = 0.4*sin(2*pi/waveLength*patches.x);

```

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

```

306 u([1:2 end-1:end],:) = nan;
307 patches.i = find(~isnan(u));

```

Seek the equilibrium, and report the norm of the residual, via the generic patch system wrapper `theRes` (Section 3.18.2).

```

315 tic
316 [u(patches.i),res] = fsolve(@(v) theRes(v,patches,k0,Ra,1) ...
317 ,u(patches.i) ,optimoptions('fsolve','Display','off'));
318 solveTime = toc
319 normRes = norm(res)
320 if normRes>1e-7, warning('residual large: bad equilibrium'),end

```

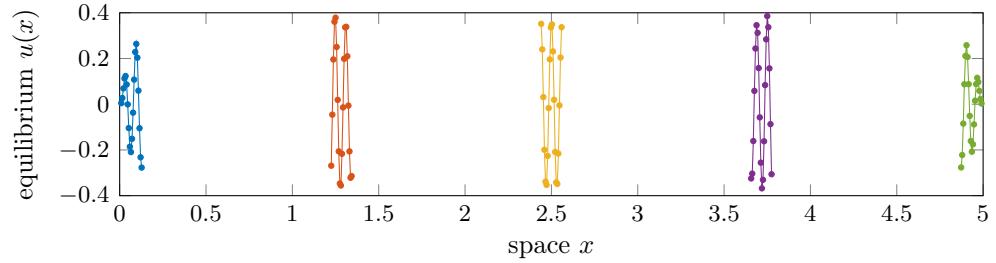
Plot the equilibrium see Figure 3.35.

```

328 figure(1),clf
329 subplot(2,1,1)
330 plot(xs,squeeze(u),'.-')
331 xlabel('space $x$'),ylabel('equilibrium $u(x)$')
332 ifOurCf2tex([basename 'Equilib'])%optionally save

```

Figure 3.35: an equilibrium of the heterogeneous Swift–Hohenberg PDE determined by the patch scheme



3.18.0.3 Simulate in time

Set an initial condition, and here integrate forward in time using a standard method for stiff systems—because of the simplicity of linear problems this method works quite efficiently here. Integrate the interface `patchSys1` (Section 3.2) to the microscale differential equations.

```

357 fprintf('**** Simulate in time\n')
358 u0 = 0*sin(2*pi/waveLength*patches.x)+0.1*randn(nSubP,1,1,nPatch);
359 tic
360 [ts,us] = ode15s(@patchSys1, [0 40], u0(:),[], patches,k0,Ra,1);
361 simulateTime = toc
362 us = reshape(us,length(ts),numel(patches.x(:)),[]);

```

Plot the simulation in Figure 3.31.

```

369 figure(2),clf
370 xs([1:2 end-1:end],:) = nan;
371 mesh(ts(1:3:end),xs(:,us(1:3:end,:))), view(65,60)
372 colormap(0.7*hsv)
373 xlabel('time $t$'), ylabel('space $x$'), zlabel('$u(x,t)$')
374 ifOurCf2eps([basename 'Uxt'])

```

Fin.

3.18.1 Heterogeneous SwiftHohenberg PDE+BCs inside patches

As a microscale discretisation of Swift–Hohenberg PDE $u_t = -D[c_1(x)Du] + Ra u - u^3$, where heterogeneous operator $D = 1 + \partial_x(c_2(x)\partial_x)/k_0^2$.

```

388 function ut=heteroSwiftHohenbergPDE(t,u,patches,k0,Ra,cubic)
389     dx=diff(patches.x(1:2)); % microscale spacing
390     i=3:size(u,1)-2; % interior points in patches

```

Code a couple of different boundary conditions of zero function and derivative(s) at left-end of left-patch, and right-end of right-patch. For slightly simpler coding, squeeze out the two singleton dimensions.

```

399     u = squeeze(u);
400     if ~patches.periodic
401         switch 1

```

```

402      case 1 % these are u=u_x=0
403          u(1:2,1)=0;
404          u(end-1:end,end)=0;
405      case 2 % these are u=u_xx=0
406          u(1:2,1) = [-u(3,1); 0];
407          u(end-1:end,end) = [0; -u(end-2,end)];
408      end% case
409  end%if

```

Here code straightforward centred discretisation in space.

```

415  ut = nan+u;           % preallocate output array
416  v = u(2:end-1,:)+diff(patches.cs(:,2).*diff(u))/dx^2/k0^2;
417  v = v.*patches.cs(2:end,1);
418  v = v(2:end-1,:)+diff(patches.cs(2:end-1,2).*diff(v))/dx^2/k0^2;
419  ut(i,:) = -v +Ra*u(i,:) -cubic*u(i,:).^3;
420  end

```

3.18.2 theRes(): a wrapper function

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

```

435  function f=theRes(u,patches,k0,Ra,cubic)
436      v=nan(size(patches.x));
437      v(patches.i) = u;
438      f = patchSys1(0,v(:,),patches,k0,Ra,cubic);
439      f = f(patches.i);
440  end%function theRes

```

3.19 theRes(): wrapper function to zero for equilibria

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.

```
15 function f=theRes(u)
16     global patches
17     switch numel(size(patches.x))
18         case 4, pSys = @patchSys1;
19             v=nan(size(patches.x));
20         case 5, pSys = @patchSys2;
21             v=nan(size(patches.x+patches.y));
22         case 6, pSys = @patchSys3;
23             v=nan(size(patches.x+patches.y+patches.z));
24         otherwise error('number of dimensions is somehow wrong')
25     end%switch
26     v(patches.i) = u;
27     f = pSys(1,v(:,),patches);
28     f = f(patches.i);
29 end%function theRes
```

3.20 quasiLogAxes(): transforms some axes of a plot to quasi-log

This function rescales some coordinates and labels the axes of the given 2D or 3D plot. The original aim was to effectively show the complex spectrum of multiscale systems such as the patch scheme. The eigenvalues are over a wide range of magnitudes, but are signed. So we use a nonlinear asinh transformation of the axes, and then label the axes with reasonable ticks. The nonlinear rescaling is useful in other scenarios also.

```
21 function quasiLogAxes(handle,xScale,yScale,zScale,cScale)
```

Input

- **handle**: handle to your plot to transform, for example, obtained by `handle=plot(...)`
- **xScale** (optional, default inf): if inf, then no transformation is done in the ‘x’-coordinate. Otherwise, when **xScale** is not inf, transforms the plot *x*-coordinates with the `asinh()` function so that
 - for $|x| \lesssim x_{\text{scale}}$ the x-axis scaling is approximately linear, whereas
 - for $|x| \gtrsim x_{\text{scale}}$ the x-axis scaling is approximately signed-logarithmic.
- **yScale** (optional, default inf): corresponds to **xScale** for the second axis scaling.
- **zScale** (optional, default inf): corresponds to **xScale** for a third axis scaling if it exists.
- **cScale** (optional, default inf): corresponds to **xScale** but for a colormap, and colorbar scaling if one exists.

Output

None, just the transformed plot.

Example If invoked with no arguments, then execute an example.

```
58 if nargin==0
59     % generate some data
60     n=99; fast=(rand(n,1)<0.8);
61     z = -rand(n,1).*(1+1e3*fast)+1i*randn(n,1).*(5+1e2*fast);
62     % plot data and transform axes
63     handle = plot(real(z),imag(z),'.');
64     xlabel('real-part'), ylabel('imag-part')
65     quasiLogAxes(handle,1,10);
66     return
67 end% example
```

Default values for scaling, `inf` denotes no transformation of that axis.

```
76 if nargin<5, cScale=inf; end
77 if nargin<4, zScale=inf; end
78 if nargin<3, yScale=inf; end
79 if nargin<2, xScale=inf; end
```

Get current limits of the plot to use if the user has set them already. And also get the pointer to the axes and to the figure of the plot.

```
90  xlim0=xlim; ylim0=ylim; zlim0=zlim; clim0=caxis;
91  theAxes = get(handle(1),'parent');
92  theFig = get(theAxes,'parent');
```

Find overall factors so the data is nonlinearly mapped to order oneish—so that then pgfplots et al. do not think there is an overall scaling factor on the axes.

```
101 xFac=1e-99; yFac=xFac; zFac=xFac; cFac=xFac;
102 for k=1:length(handle)
103     if ~isinf(xScale)
104         temp = asinh(handle(k).XData/xScale);
105         xFac = max(xFac, max(abs(temp(:)),[],'omitnan') );
106     end
107     if ~isinf(yScale)
108         temp = asinh(handle(k).YData/yScale);
109         yFac = max(yFac, max(abs(temp(:)),[],'omitnan') );
110     end
111     if ~isinf(zScale)
112         temp = asinh(handle(k).ZData/zScale);
113         zFac = max(zFac, max(abs(temp(:)),[],'omitnan') );
114     end
115     if ~isinf(cScale)
116         temp = asinh(handle(k).CData/cScale);
117         cFac = max(cFac, max(abs(temp(:)),[],'omitnan') );
118     end
119 end%for
120 xFac=9/xFac; yFac=9/yFac; zFac=9/zFac; cFac=9/cFac;
```

Scale the plot data in the plot handle. Give an error if it appears that the plot-data has already been transformed. Color data has to be transformed first because usually there is automatic flow from z-data to c-data.

```
130 for k=1:length(handle)
131     assert(~strcmp(handle(k).UserData,'quasiLogAxes'), ...
132             'Replot graph---it appears plot data is already transformed')
133     if ~isinf(cScale)
134         handle(k).CData = cFac*asinh(handle(k).CData/cScale);
135         clim1=[min(handle(k).CData(:)) max(handle(k).CData(:))];
136     end
137     if ~isinf(xScale)
138         handle(k).XData = xFac*asinh(handle(k).XData/xScale);
139         xlim1=[min(handle(k).XData(:)) max(handle(k).XData(:))];
140     end
141     if ~isinf(yScale)
142         handle(k).YData = yFac*asinh(handle(k).YData/yScale);
143         ylim1=[min(handle(k).YData(:)) max(handle(k).YData(:))];
144     end
```

```

145      if ~isinf(zScale)
146          handle(k).ZData = zFac*asinh(handle(k).ZData/zScale);
147          zlim1=[min(handle(k).ZData(:)) max(handle(k).ZData(:))];
148      end
149      handle(k).UserData = 'quasiLogAxes';
150  end%for

```

Set 4% padding around all margins of transformed data—crude but serviceable. Unless the axis had already been manually set, in which case use the transformed set limits.

```

159  if ~isinf(xScale),
160      if xlim('mode')=="manual"
161          xlim1=xFac*asinh(xlim0/xScale);
162      else xlim1=xlim1+0.04*diff(xlim1)*[-1 1];
163      end, end
164  if ~isinf(yScale),
165      if ylim('mode')=="manual"
166          ylim1=yFac*asinh(ylim0/yScale);
167      else ylim1=ylim1+0.04*diff(ylim1)*[-1 1];
168      end, end
169  if ~isinf(zScale),
170      if zlim('mode')=="manual"
171          zlim1=zFac*asinh(zlim0/zScale);
172      else zlim1=zlim1+0.04*diff(zlim1)*[-1 1];
173      end, end
174  if ~isinf(cScale),
175      if theAxes.CLimMode=="manual"
176          clim1=cFac*asinh(clim0/cScale);
177      else clim1=clim1+ 0*diff(clim1)*[-1 1];
178      end, end

```

Scale axes, and tick marks on axes

```

186  if ~isinf(xScale)
187      xlim(xlim1);
188      tickingQuasiLogAxes(theAxes,'X',xlim1,xScale,xFac)
189  end%if
190  if ~isinf(yScale)
191      ylim(ylim1);
192      tickingQuasiLogAxes(theAxes,'Y',ylim1,yScale,yFac)
193  end%if
194  if ~isinf(zScale)
195      zlim(zlim1);
196      tickingQuasiLogAxes(theAxes,'Z',zlim1,zScale,zFac)
197  end%if

```

But for color, only tick when we find a colorbar.

```

203  if ~isinf(cScale)
204      caxis(clim1);

```

```

205     for p=1:numel(theFig.Children)
206         ca = theFig.Children(p);
207         if class(ca) == "matlab.graphics.illustration.ColorBar"
208             tickingQuasiLogAxes(ca,'C',clim1,cScale,cFac)
209             break
210         end
211     end
212 end%if

Turn the grid on by default.

218 grid on
219 end%function

```

3.20.1 tickingQuasiLogAxes(): typeset ticks and labels on an axis

```
228 function tickingQuasiLogAxes(ca,Q,qlim1,qScale,qFac)
```

Input

- ca: pointer to axes/colorbar dataset.
- Q: character, either X, Y, Z, C.
- qlim1: the scaled limits of the axis.
- qScale: the scaling parameter for the axis.
- qFac: the scaling factor for the axis.

Output

None, just the ticked and labelled axes.

Get the order of magnitude of the horizontal data.

```

245 qmax=max(abs(qlim1));
246 qmag=floor(log10(qScale*sinh(qmax/qFac)));

```

Form a range of ticks, geometrically spaced, trim off the small values that would be too dense near zero (omit those within 6% of qmax).

```

254 ticks=10.^(-qmag+(-7:0));
255 j=find(ticks>qScale*sinh(0.06*qmax/qFac));
256 nj=length(j);
257 if nj<3,    ticks=[1;2;5]*ticks(j);
258 elseif nj<5, ticks=[1;3]*ticks(j);
259 else        ticks=ticks(j);
260 end
261 ticks=sort([0;ticks(:);-ticks(:)]);

```

Set the ticks in place according to the transformation.

```

267 if Q=='C', p='s'; Q=''; else p=''; end
268 set(ca,[Q 'Tick' p],qFac*asinh(ticks/qScale) ...
269 , [Q 'TickLabel' p],cellstr(num2str(ticks,4)))

```

```

270      if Q=='X', set(ca,[Q 'TickLabelRotation'],40), end
271  end%function qScaling

```

3.20.2 patchEdgeInt1test: test the 1D patch coupling

A script to test the spectral and finite-order polynomial interpolation of function `patchEdgeInt1()`. Tests one or several variables, normal and staggered grids, and also tests centre and edge interpolation. But does not yet test core averaging, nor divided differences on staggered, etc.

Start by establishing global data struct, and the number of realisations of cases.

```

22 clear all, close all
23 global patches
24 nRealise = 20

```

3.20.2.1 Check divided difference interpolation

```

36 fprintf('\n\n**** Check divided difference interpolation\n')
37 pause(1)

```

But not yet implemented staggered grid version?? Check over various types and orders of interpolation, numbers of patches, random domain lengths, random ratios, and randomised distribution of patches. (The `@sin` is a dummy.)

```

47 for iReal=1:nRealise
48     nEdge = randi(3)% =1,2, or 3
49     edgyInt = rand<0.5
50     nSubP = nEdge*( (2-edgyInt)*randi(2)+1+edgyInt )
51     ordCC = 2*randi(4)
52     nPatch = ordCC+randi([2 4])
53     Domain=5*[-rand rand]
54     dx=rand*diff(Domain)/nPatch/nSubP
55     configPatches1(@sin,Domain,'equispace',nPatch,ordCC,dx,nSubP ...
56         , 'EdgyInt',edgyInt,'nEdge',nEdge);
57     patches.intTest = true;

```

Displace patches to a random non-uniform spacing.

```

63 H = diff(patches.x(:,:,1:2));
64 patches.x = patches.x+0.8*H*(rand(1,1,1,nPatch)-0.5);
65 %H = squeeze( diff(patches.x(:,:,1)) )% for information only

```

Check multiple fields simultaneously Set profiles to be various powers of x , ps , and store as different ‘variables’ at each point.

```

76 ps=1:ordCC
77 cs=randn(size(ps));
78 u0=patches.x.^ps.*cs+randn;

```

Copy data, and set edges to `inf` so we can be certain that interpolation is computing the required edge values.

```
85      u=u0;  u([1:nEdge  end-nEdge+1:end],:)=inf;
```

Then evaluate the interpolation and squeeze the singleton dimension of an ‘ensemble’.

```
92      ui=patchEdgeInt1(u(:));
93      ui=squeeze(ui);
```

All patches should have zero error: but need to either in `patchEdgeInt1` comment out NaN assignment of boundary values, or not test the two extreme patches here, or add code to omit NaNs here. High-order interpolation seems to be more affected by round-off so relax error size.

```
103     j=1:nPatch;
104     iError=ui(:,:,j)-u0(:,:,j);
105     hist(log10(abs(iError(abs(iError)>0))),-17:-9)
106     xlabel('log10 iError'), pause(0.3)%%
107     normError=norm(iError(:))
108     assert(normError<1e-13*4^ordCC ...
109     , 'failed divided difference interpolation')
```

End the for-loop over random parameters.

```
116 end%for iReal
117 fprintf('\n\nPassed all divided difference interpolation\n')
```

3.20.2.2 Test standard spectral interpolation

```
133 fprintf('\n\n**** Test standard spectral interpolation\n')
134 pause(1)
```

Test over random numbers of patches, random domain lengths, random microscale spacing, random choice of `edgyInt`. Say do fifteen realisations.

```
142 for iReal=1:nRealise
143     nEdge=randi(3)% =1,2, or 3
144     edgyInt = rand<0.5
145     nSubP = nEdge*( (2-edgyInt)*randi(2)+1+edgyInt )
146     nPatch=randi([5 10])
147     Len=10*rand
148     dx=0.5*rand*Len/nPatch/nSubP
149     configPatches1(@sin,[0 Len],'periodic',nPatch,0,dx,nSubP ...
150     , 'EdgyInt',edgyInt,'nEdge',nEdge); % random Edgy or not
151     if mod(nPatch,2)==0, fprintf('\nAvoiding highest wavenumber\n'), end
152     kMax=floor((nPatch-1)/2);
```

Test single field Set a profile, and evaluate the interpolation.

```
160 for k=-kMax:kMax
161     u0=exp(1i*k*patches.x*x2*pi/Len);
```

```

162     u=u0;  u([1:nEdge  end-nEdge+1:end],:)=nan;
163     ui=patchEdgeInt1(u(:));
164     normError=rms(ui(:)-u0(:));
165     if abs(normError)>5e-14
166         normError=normError, k=k
167         error(['failed single var interpolation k=' num2str(k)])
168     end
169 end

```

Test multiple fields Use this to measure some of the errors in order to omit singleton dimensions,

```

177     normDiff=@(u,v) ...
178     norm(squeeze(u)-squeeze(v));%*norm(squeeze(v(i0,:,:,:)));

```

Set a profile, and evaluate the interpolation. For the case of the highest wavenumber, squash the error when the centre-patch values are all zero by multiplying by result norm. Not yet working for edgy interpolation.

```

188 for k=1:(nPatches-1)/2 % not checking the highest wavenumber
189     u0=sin(k*patches.x*2*pi/Len);
190     v0=cos(k*patches.x*2*pi/Len);
191     uvi=patchEdgeInt1( reshape([u0 v0],[],1) );
192     normuError=normDiff(uvi(:,1,:,:),u0);
193     normvError=normDiff(uvi(:,2,:,:),v0);
194     if abs(normuError)+abs(normvError)>2e-13
195         normuError=normuError, normvError=normvError
196         error(['failed double field interpolation k=' num2str(k)])
197     end
198 end

```

End the for-loop over various geometries.

```

205 end
206 fprintf('\nPassed standard spectral interpolation tests\n')

```

3.20.2.3 Now test spectral interpolation on staggered grid

```

221 fprintf('\n\n**** Test spectral interpolation on staggered\n')
222 pause(1)

```

Must have even number of patches for a staggered grid. Have not yet implemented multiple edge values for a staggered grid as I am uncertain whether it makes any sense—certainly this test fails anyway.

```

231 for iReal=1:nRealise
232     nEdge = 1 % required
233     edgyInt = rand<0.5
234     nPatch=2*randi([3 10])
235     nSubP=7 % of form 4*N-1
236     Len=10*rand
237     dx=0.5*rand*Len/nPatch/nSubP

```

```

238     configPatches1(@simpleWavePde,[0 Len], 'periodic' ...
239             ,nPatch,-1,dx,nSubP,'EdgyInt',edgyInt,'nEdge',nEdge);
240     if mod(nPatch,4)==0, fprintf('\nAvoiding highest wavenumber\n'), end
241     kMax=floor((nPatch/2-1)/2)

```

Identify which microscale grid points are h or u values.

```

247 uPts=mod( (1:nSubP)+(1:nPatch) ,2);
248 hPts=find(1-uPts);
249 uPts=find(uPts);

```

Set a profile for various wavenumbers. The capital letter U denotes an array of values merged from both u and h fields on the staggered grids.

```

257 fprintf('Staggered: single field-pair test.\n')
258 for k=-kMax:kMax
259     U0=nan(nSubP,nPatch);
260     U0(hPts)=rand*exp(+1i*k*patches.x(hPts)*2*pi/Len);
261     U0(uPts)=rand*exp(-1i*k*patches.x(uPts)*2*pi/Len);
262     U=U0;
263     U([1:nEdge end-nEdge+1:end],:)=nan;
264     Ui=patchEdgeInt1(U0(:));
265     normError=norm(Ui(:)-U0(:));
266     if abs(normError)>5e-14
267         normError=normError
268         patches=patches
269         error(['staggered: failed single sys interpolation k=' num2str(k)])
270     end
271 end

```

Test multiple fields Use this to measure some of the errors in order to omit singleton dimensions, and also squish any errors if the third argument is essential zero (to cater for cosine aliasing errors).

```

282 normDiff=@(u,v,w) ...
283 norm(squeeze(u)-squeeze(v));%*norm(squeeze(w(i0,:,:,:)));

```

Set a profile, and evaluate the interpolation. For the case of the highest wavenumber zig-zag, squash the error when the alternate centre-patch values are all zero. First shift the x -coordinates so that the zig-zag mode is centred on a patch.

```

293 fprintf('Staggered: Two field-pairs test.\n')
294 x0=patches.x((nSubP+1)/2,1);
295 patches.x=patches.x-x0;
296 oddP=1:2:nPatch; evnP=2:2:nPatch;
297 for k=1:kMax
298     U0=nan(nSubP,1,1,nPatch); V0=U0;
299     U0(hPts)=rand*sin(k*patches.x(hPts)*2*pi/Len);
300     U0(uPts)=rand*sin(k*patches.x(uPts)*2*pi/Len);
301     U=U0; U([1:nEdge end-nEdge+1:end],:)=nan;
302     V0(hPts)=rand*cos(k*patches.x(hPts)*2*pi/Len);

```

```

303     V0(uPts)=rand*cos(k*patches.x(uPts)*2*pi/Len);
304     V=V0; V([1:nEdge end-nEdge+1:end],:)=nan;
305     UVi=patchEdgeInt1([U0 V0]);
306     normuError=[normDiff(UVi(:,1,:,:oddP),U0(:,:,:oddP),U0(:,:,:evenP))
307                  normDiff(UVi(:,1,:,:evenP),U0(:,:,:evenP),U0(:,:,:oddP))]';
308     normvError=[normDiff(UVi(:,2,:,:oddP),V0(:,:,:oddP),V0(:,:,:evenP))
309                  normDiff(UVi(:,2,:,:evenP),V0(:,:,:evenP),V0(:,:,:oddP))]';
310     if norm(normuError)+norm(normvError)>2e-13
311         normuError=normuError, normvError=normvError
312         patches=patches
313         error(['staggered: failed double field interpolation k=' num2str(k)])
314     end
315 end

End for-loop over patches

322 end

```

3.20.2.4 Check standard finite width interpolation

```

336 fprintf('\n\n**** Check standard finite width interpolation\n')
337 pause(1)

```

Check over various types and orders of interpolation, numbers of patches, random domain lengths and random ratios. (The @sin is a dummy.)

```

345 for iReal=1:nRealise
346     nEdge=randi(3)% =1,2, or 3
347     edgyInt = rand<0.5
348     nSubP = nEdge*( (2-edgyInt)*randi(2)+1+edgyInt )
349     ordCC = 2*randi(4)
350     nPatch = ordCC+randi([2 4])
351     Domain=5*[-rand rand]
352     dx=0.5*rand*diff(Domain)/nPatch/nSubP
353     configPatches1(@sin,Domain,'periodic',nPatch,ordCC,dx,nSubP ...
354                   , 'EdgyInt',edgyInt,'nEdge',nEdge);

```

Check multiple fields simultaneously Set profiles to be various powers of x , ps , and store as different ‘variables’ at each point.

```

363     ps=1:ordCC
364     cs=randn(size(ps));
365     u0=patches.x.^ps.*cs+randn;

```

Copy data, and set edges to NaN so we can be certain that interpolation is computing the required edge values.

```

372     u=u0; u([1:nEdge end-nEdge+1:end],:)=nan;

```

Then evaluate the interpolation and squeeze the singleton dimension of an ‘ensemble’.

```

379     ui=patchEdgeInt1(u(:));
380     ui=squeeze(ui);

```

The interior patches should have zero error.

```

386     j=ordCC/2+1:nPatch-ordCC/2;
387     iError=ui(:,:,j)-u0(:,:,j);
388     normError=norm(iError(:))
389     assert(normError<5e-12 ...
390         , 'failed finite stencil interpolation')

```

End the for-loops over various parameters.

```

397 end%for iReal
398 fprintf('\nPassed all standard polynomial interpolation\n')

```

3.20.2.5 Now test finite width interpolation on staggered grid

```

413 fprintf('\n\n**** Check finite width staggered\n')
414 pause(1)

```

Must have even number of patches for a staggered grid.

```

420 for iReal=1:nRealise
421     nEdge = 1 % required for now
422     edgyInt = rand<0.5
423     nPatch=2*randi([3 10])
424     nSubP=3; % of form 4*N-1
425     Len=10*rand
426     dx=0.5*rand*Len/nPatch/nSubP
427     configPatches1(@simpleWavepde,[0 Len], 'periodic' ...
428                 ,nPatch,-1,dx,nSubP,'EdgyInt',edgyInt,'nEdge',nEdge);
429     kMax=floor((nPatch/2-1)/2)

```

Identify which microscale grid points are h or u values.

```

436 uPts=mod( (1:nSubP)'+(1:nPatch) ,2);
437 hPts=find(1-uPts);
438 uPts=find(uPts);

```

Set a profile for various wavenumbers. The capital letter U denotes an array of values merged from both u and h fields on the staggered grids.

```

446 fprintf('\nSingle field-pair test.\n')
447 for k=-kMax:kMax
448     U0=nan(nSubP,nPatch);
449     U0(hPts)=rand*exp(+1i*k*patches.x(hPts)*2*pi/Len);
450     U0(uPts)=rand*exp(-1i*k*patches.x(uPts)*2*pi/Len);
451     Ui=squeeze(patchEdgeInt1(U0(:)));
452     normError=norm(Ui-U0);
453     if abs(normError)>5e-14
454         normError=normError
455         error(['failed single sys interpolation k=' num2str(k)])

```

```

456     end
457 end

```

Test multiple fields Set a profile, and evaluate the interpolation. For the case of the highest wavenumber zig-zag, squash the error when the alternate centre-patch values are all zero. First shift the x -coordinates so that the zig-zag mode is centred on a patch.

```

469 i0=(nSubP+1)/2; % centre-patch index
470 fprintf('Two field-pairs test.\n')
471 x0=patches.x((nSubP+1)/2,1);
472 patches.x=patches.x-x0;
473 for k=1:nPatch/4
474     U0=nan(nSubP,1,1,nPatch); V0=U0;
475     U0(hPts)=rand*sin(k*patches.x(hPts)*2*pi/Len);
476     U0(uPts)=rand*sin(k*patches.x(uPts)*2*pi/Len);
477     V0(hPts)=rand*cos(k*patches.x(hPts)*2*pi/Len);
478     V0(uPts)=rand*cos(k*patches.x(uPts)*2*pi/Len);
479     UVi=patchEdgeInt1([U0 V0]);
480     Ui=squeeze(UVi(:,1,1,:));
481     Vi=squeeze(UVi(:,2,1,:));
482     normuError=norm(Ui(:,1:2:nPatch)-U0(:,1:2:nPatch))*norm(U0(i0,2:2:nPatch))
483         +norm(Ui(:,2:2:nPatch)-U0(:,2:2:nPatch))*norm(U0(i0,1:2:nPatch));
484     normvError=norm(Vi(:,1:2:nPatch)-V0(:,1:2:nPatch))*norm(V0(i0,2:2:nPatch))
485         +norm(Vi(:,2:2:nPatch)-V0(:,2:2:nPatch))*norm(V0(i0,1:2:nPatch));
486     if abs(normuError)+abs(normvError)>2e-13
487         normuError=normuError, normvError=normvError
488         error(['failed double field interpolation k=' num2str(k)])
489     end
490 end
End for-loop over the realisations
497 end

```

3.20.2.6 Finish

If no error messages, then all OK.

```

509 fprintf('\n**** If you read this, then all tests were passed\n')

```

4 Patches in 2D space

4.1 configPatches2(): configures spatial patches in 2D

Section contents

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Makes the struct `patches` for use by the patch/gap-tooth time derivative/step function `patchSys2()`. [Section 4.1.1](#) lists an example of its use.

```
19 function patches = configPatches2(fun,Xlim,Dom ...
20     ,nPatch,ordCC,dx,nSubP,varargin)
21 version = '2023-04-12';
```

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 4.1.1](#) for an example code.

- `fun` is the name of the user function, `fun(t,u,patches)` or `fun(t,u)` or `fun(t,u,patches,...)`, 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 $[Xlim(1), Xlim(2)] \times [Xlim(3), Xlim(4)]$. 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, . . . ; 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—adjusted a little when `nEdge > 1`. So either `ratio = ½` 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 `nSubP./nEdge` must be odd integer(s) so that there is/are centre-patch lattice lines. So for the defaults of `nEdge = 1` and not `EdgyInt`, then `nSubP` must be odd.
- ‘`nEdge`’, *optional* (integer—scalar or two element), default=1, the width of edge values set by interpolation at the edge regions of each patch. If two elements, then respectively the width in x, y -directions. 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. Best accuracy usually obtained when the periodicity of the coefficients is a factor of **nSubP-2*nEdge** for **EdgyInt**, or a factor of $(\text{nSubP}-\text{nEdge})/2$ for not **EdgyInt**.
 - 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.¹

```
213 if nargout==0, global patches, end
214 patches.version = version;
```

¹ 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)` or `fun(t,u,patches,...)`, 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 `.Cwts1`, only for macro-periodic conditions, are the `ordCC` × 2-array of weights for the inter-patch interpolation onto the right/top and left/bottom edges (respectively) with patch:macroscale ratio as specified or as derived from `dx`.
- `.x` (6D) is `nSubP(1) × 1 × 1 × 1 × nPatch(1) × 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` 1×2 , is the width of edge values set by interpolation at the edge regions of each patch, in the x, y -directions respectively.
- `.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.

4.1.1 If no arguments, then execute an example

```

298 if nargin==0
299 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 et al. \(2014\)](#) established that this scheme is consistent with the PDE (as the patch spacing decreases).

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

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

```
331 u0 = exp(-patches.x.^2-patches.y.^2);
332 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.

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

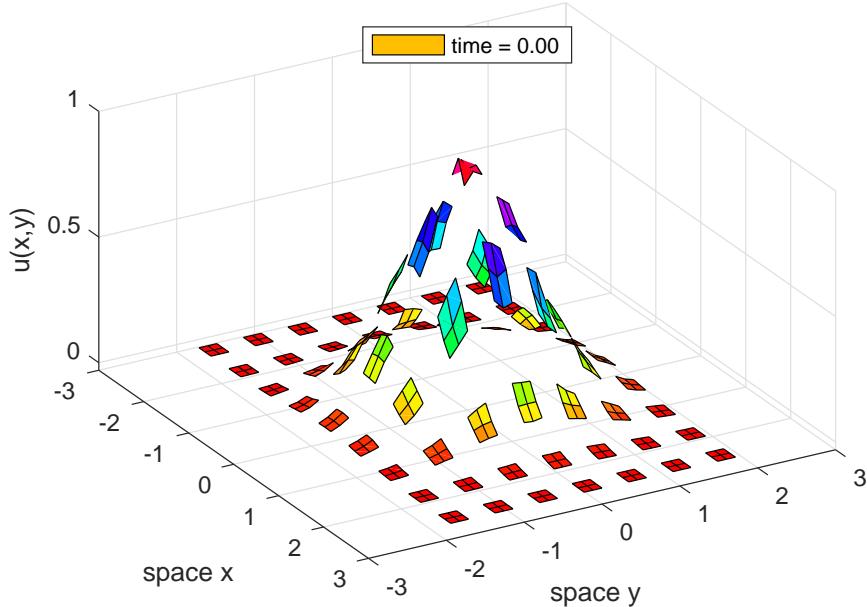
Start by showing the initial conditions of [Figure 4.1](#) while the simulation computes.

```
349 u = reshape(permute(squeeze(u0) ...
350     ,[1 3 2 4]), [numel(x) numel(y)]);
351 hsurf = mesh(x(:, ), y(:, ), u');
352 axis([-3 3 -3 3 -0.03 1]), view(60,40)
353 legend('time = 0.00', 'Location', 'north')
354 xlabel('space $x$'), ylabel('space $y$'), zlabel('$u(x,y)$')
355 colormap(hsv)
356 ifOrCf2eps([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 et al. 2020](#), Fig. 4). Ask for output at non-uniform times because the diffusion slows.

```
373 disp('Wait to simulate nonlinear diffusion h_t=(h^3)_xx+(h^3)_yy')
374 drawnow
375 if ~exist('OCTAVE_VERSION', 'builtin')
376     [ts,us] = ode23(@patchSys2,linspace(0,2).^2,u0(:));
377 else % octave version is quite slow for me
```

Figure 4.1: initial field $u(x, y, t)$ at time $t = 0$ of the patch scheme applied to a nonlinear ‘diffusion’ PDE: Figure 4.2 plots the computed field at time $t = 3$.



```

378     lsode_options('absolute tolerance',1e-4);
379     lsode_options('relative tolerance',1e-4);
380     [ts,us] = ode0cts(@patchSys2,[0 1],u0(:));
381 end

```

Animate the computed simulation to end with Figure 4.2. Use `patchEdgeInt2` to interpolate patch-edge values.

```

389 for i = 1:length(ts)
390     u = patchEdgeInt2(us(i,:));
391     u = reshape(permute(squeeze(u) ...
392                 ,[1 3 2 4]), [numel(x) numel(y)]);
393     set(hsurf,'ZData', u');
394     legend(['time = ' num2str(ts(i),'%4.2f')])
395     pause(0.1)
396 end
397 if0urCf2eps([mfilename 't3'])

```

Upon finishing execution of the example, exit this function.

```

412 return
413 end%if no arguments

```

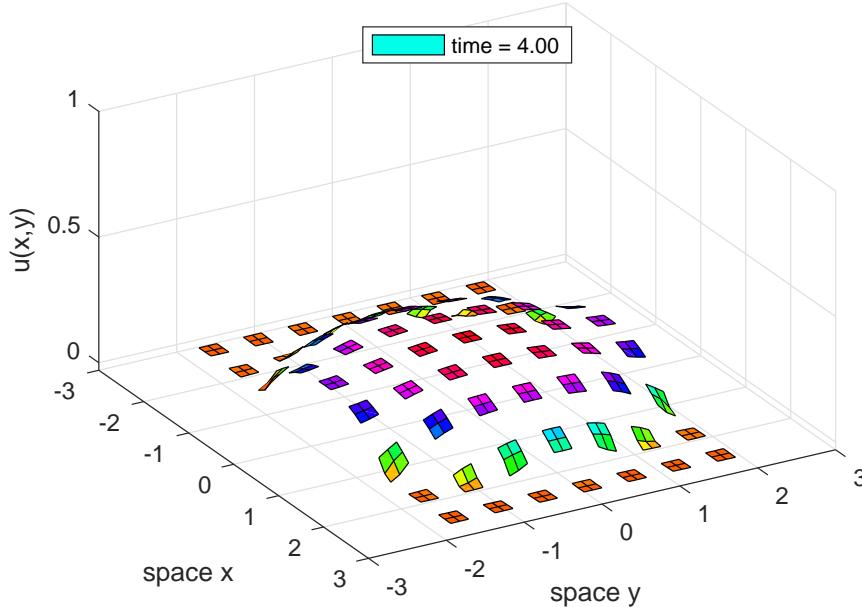
Example of nonlinear diffusion PDE inside patches As a microscale discretisation of $u_t = \nabla^2(u^3)$, code $\dot{u}_{ijkl} = \frac{1}{\delta x^2}(u_{i+1,j,k,l}^3 - 2u_{i,j,k,l}^3 + u_{i-1,j,k,l}^3) + \frac{1}{\delta y^2}(u_{i,j+1,k,l}^3 - 2u_{i,j,k,l}^3 + u_{i,j-1,k,l}^3)$.

```

13 function ut = nonDiffPDE(t,u,patches)
14     if nargin<3, global patches, end
15     u = squeeze(u); % reduce to 4D

```

Figure 4.2: field $u(x, y, t)$ at time $t = 3$ of the patch scheme applied to a nonlinear ‘diffusion’ PDE with initial condition in Figure 4.1.



```

16     dx = diff(patches.x(1:2)); % microgrid spacing
17     dy = diff(patches.y(1:2));
18     i = 2:size(u,1)-1; j = 2:size(u,2)-1; % interior patch points
19     ut = nan+u; % preallocate output array
20     ut(i,j,:,:,:) = diff(u(:,j,:,:,:).^3,2,1)/dx^2 ...
21                     +diff(u(i,:,:,:, :).^3,2,2)/dy^2;
22   end

```

4.1.2 Parse input arguments and defaults

```

427 p = inputParser;
428 fnValidation = @(f) isa(f, 'function_handle');%test for fn name
429 addRequired(p, 'fun',fnValidation);
430 addRequired(p, 'Xlim',@isnumeric);
431 %addRequired(p, 'Dom'); % nothing yet decided
432 addRequired(p, 'nPatch',@isnumeric);
433 addRequired(p, 'ordCC',@isnumeric);
434 addRequired(p, 'dx',@isnumeric);
435 addRequired(p, 'nSubP',@isnumeric);
436 addParameter(p, 'nEdge',1,@isnumeric);
437 addParameter(p, 'EdgyInt',false,@islogical);
438 addParameter(p, 'nEnsem',1,@isnumeric);
439 addParameter(p, 'hetCoeffs',[],@isnumeric);
440 addParameter(p, 'parallel',false,@islogical);
441 %addParameter(p, 'nCore',1,@isnumeric); % not yet implemented
442 parse(p,fun,Xlim,nPatch,ordCC,dx,nSubP,varargin{:});

```

Set the optional parameters.

```

448 patches.nEdge = p.Results.nEdge;
449 if numel(patches.nEdge)==1
450     patches.nEdge = repmat(patches.nEdge,1,2);
451 end
452 patches.EdgyInt = p.Results.EdgyInt;
453 patches.nEnsem = p.Results.nEnsem;
454 cs = p.Results.hetCoeffs;
455 patches.parallel = p.Results.parallel;
456 %patches.nCore = p.Results.nCore;

```

Initially duplicate parameters for both space dimensions as needed.

```

464 if numel(Xlim)==2, Xlim = repmat(Xlim,1,2); end
465 if numel(nPatch)==1, nPatch = repmat(nPatch,1,2); end
466 if numel(dx)==1, dx = repmat(dx,1,2); end
467 if numel(nSubP)==1, nSubP = repmat(nSubP,1,2); end

```

Check parameters.

```

474 assert(Xlim(1)<Xlim(2) ...
475     , 'first pair of Xlim must be ordered increasing')
476 assert(Xlim(3)<Xlim(4) ...
477     , 'second pair of Xlim must be ordered increasing')
478 assert((mod(ordCC,2)==0)|all(patches.nEdge==1) ...
479     , 'Cannot yet have nEdge>1 and staggered patch grids')
480 assert(all(3*patches.nEdge<=nSubP) ...
481     , 'too many edge values requested')
482 assert(all(rem(nSubP,patches.nEdge)==0) ...
483     , 'nSubP must be integer multiple of nEdge')
484 if ~patches.EdgyInt, assert(all(rem(nSubP./patches.nEdge,2)==1) ...
485     , 'for non-edgyInt, nSubP./nEdge must be odd integer')
486 end
487 if (patches.nEnsem>1)&all(patches.nEdge>1)
488     warning('not yet tested when both nEnsem and nEdge non-one')
489 end
490 %if patches.nCore>1
491 %    warning('nCore>1 not yet tested in this version')
492 %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.

```

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

```

Default macroscale conditions are periodic with evenly spaced patches.

```

513 if isempty(Dom), Dom=struct('type','periodic'); end
514 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.

```
522 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.

```
535 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.

```
544 patches.periodic=false;
545 for p=1:2
546 switch Dom.type(p,:)
547 case 'periodic'
548     patches.periodic=true;
549     if isfield(Dom,'bcOffset')
550         warning('bcOffset not available for Dom.type = periodic'), end
551         msg=' not available for Dom.type = periodic';
552         if isfield(Dom,'X'), warning(['X' msg]), end
553         if isfield(Dom,'Y'), warning(['Y' msg]), end
554 case {'equispace','chebyshev'}
555     if ~isfield(Dom,'bcOffset'), Dom.bcOffset=zeros(2,2); end
556 % for mixed with usergiven, following should still work
557     if numel(Dom.bcOffset)==1
558         Dom.bcOffset=repmat(Dom.bcOffset,2,2); end
559     if numel(Dom.bcOffset)==2
560         Dom.bcOffset=repmat(Dom.bcOffset(:,2,1),2,1); end
561     msg=' not available for Dom.type = equispace or chebyshev';
562     if (p==1)& isfield(Dom,'X'), warning(['X' msg]), end
563     if (p==2)& isfield(Dom,'Y'), warning(['Y' msg]), end
564 case 'usergiven'
565 %     if isfield(Dom,'bcOffset')
566 %         warning('bcOffset not available for usergiven Dom.type'), end
567         msg=' required for Dom.type = usergiven';
568         if p==1, assert(isfield(Dom,'X'),['X' msg]), end
569         if p==2, assert(isfield(Dom,'Y'),['Y' msg]), end
570 otherwise
571     error(['Dom.type ' is unknown Dom.type'])
572 end%switch Dom.type
573 end%for p
```

4.1.3 The code to make patches

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

```
586 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??) -1.²

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

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

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

Check for staggered grid and periodic case.

```
613 if patches.stag, assert(all(mod(nPatch,2)==0), ...
614     'Require an even number of patches for staggered grid')
615 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.

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

Distribution depends upon `Dom.type`:

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

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

```
643 case 'periodic'
644     Q=linspace(Xlim(qq),Xlim(qq+1),nPatch(q)+1);
645     DQ=Q(2)-Q(1);
646     Q=Q(1:nPatch(q))+diff(Q)/2;
647     pEI=patches.EdgyInt; % abbreviation
648     pnE=patches.nEdge(q);% abbreviation
649     if pre2023, dx(q) = ratio(q)*DQ/(nSubP(q)-pnE*(1+pEI))*(2-pEI);
650     else         ratio(q) = dx(q)/DQ*(nSubP(q)-pnE*(1+pEI))/(2-pEI);
651     end
652     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.

```
661 case 'equispace'
662     Q=linspace(Xlim(qq)+((nSubP(q)-1)/2-Dom.bcOffset(qq))*dx(q) ...
663             ,Xlim(qq+1)-((nSubP(q)-1)/2-Dom.bcOffset(qq+1))*dx(q) ...
```

² **ToDo:** Perhaps implement staggered spectral coupling.

```

664         ,nPatch(q));
665     DQ=diff(Q(1:2));
666     width=(1+patches.EdgyInt)/2*(nSubP(q)-1-patches.EdgyInt)*dx;
667     if DQ<width*0.999999
668         warning('too many equispace patches (double overlapping)')
669     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’.³

```

686 case 'chebyshev'
687     halfWidth=dx(q)*(nSubP(q)-1)/2;
688     Q1 = Xlim(1)+halfWidth-Dom.bcOffset(qq)*dx(q);
689     Q2 = Xlim(2)-halfWidth+Dom.bcOffset(qq+1)*dx(q);
690 % 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`.

```

699 pEI=patches.EdgyInt; % abbreviation
700 pnE=patches.nEdge(q);% abbreviation
701 width=(1+pEI)/2*(nSubP(q)-pnE*(1+pEI))*dx(q);
702 for b=0:2:nPatch(q)-2
703     DQmin=(Q2-Q1-b*width)/2*( 1-cos(pi/(nPatch(q)-b-1)) );
704     if DQmin>width, break, end
705 end%for
706 if DQmin<width*0.999999
707     warning('too many Chebyshev patches (mid-domain overlap)')
708 end

```

Assign the centre-patch coordinates.

```

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

```

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

```

³ 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.

```
736 if q==1, X=Q; end
737 if q==2, Y=Q; end
738 end%for q
```

Construct the micro-grids Fourth, construct the microscale grid in each patch, centred about the given mid-points X, Y . Reshape the grid to be 6D to suit dimensions (micro,Vars,Ens,macro).

```
754 xs = dx(1)*( (1:nSubP(1))-mean(1:nSubP(1)) );
755 patches.x = reshape( xs'+X ...
756 ,nSubP(1),1,1,1,nPatch(1),1);
757 ys = dx(2)*( (1:nSubP(2))-mean(1:nSubP(2)) );
758 patches.y = reshape( ys'+Y ...
759 ,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.⁴

```
770 if patches.periodic
771     ratio = reshape(ratio,1,2); % force to be row vector
772     patches.ratio=ratio;
773     if ordCC>0
774         [Cwtsr,Cwtsl] = patchCwts(ratio,ordCC,patches.stag);
775         patches.Cwtsr = Cwtsr; patches.Cwtsl = Cwtsl;
776     end%if
777 end%if patches.periodic
```

4.1.4 Set ensemble inter-patch communication

For EdgyInt or centre interpolation respectively,

- the right-edge/centre realisations $1:n_{\text{Ensem}}$ are to interpolate to left-edge le , and
- the left-edge/centre realisations $1:n_{\text{Ensem}}$ are to interpolate to re .

re and li are ‘transposes’ of each other as $\text{re}(\text{li})=\text{le}(\text{ri})$ are both $1:n_{\text{Ensem}}$. 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()`.

```
804 nE = patches.nEnsem;
805 patches.le = 1:nE; patches.ri = 1:nE;
806 patches.bo = 1:nE; patches.to = 1:nE;
```

⁴ **ToDo:** Might sometime extend to coupling via derivative values.

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 than 3D, then the higher-dimensions are reshaped into the 3rd dimension.

```
818 if ~isempty(cs)
819     [mx,my,nc] = size(cs);
820     nx = nSubP(1); ny = nSubP(2);
821     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.

```
829 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.

```
838     patches.nEnsem = mx*my;
839     patches.cs = nan(nx-1,ny-1,nc,mx,my);
840     for j = 1:my
841         js = (j:j+ny-2);
842         for i = 1:mx
843             is = (i:i+nx-2);
844             patches.cs(:,:,i,j) = cs(is,js,:);
845         end
846     end
847     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.

```
857     le = mod((0:mx-1)+mod(nx-2,mx),mx)+1;
858     patches.le = reshape( le'+mx*(0:my-1) ,[],1);
859     ri = mod((0:mx-1)-mod(nx-2,mx),mx)+1;
860     patches.ri = reshape( ri'+mx*(0:my-1) ,[],1);
861     bo = mod((0:my-1)+mod(ny-2,my),my)+1;
862     patches.bo = reshape( (1:mx)'+mx*(bo-1) ,[],1);
863     to = mod((0:my-1)-mod(ny-2,my),my)+1;
864     patches.to = reshape( (1:mx)'+mx*(to-1) ,[],1);
```

Issue warning if the ensemble is likely to be affected by lack of scale separation.

⁵

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

⁵ **ToDo:** Maybe need to justify this and the arbitrary threshold more carefully??

End the two if-statements.

```
881     end%if-else nEnsem>1
882 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*.⁶

```
901 if patches.parallel
902 % theparpool=gcp()
903 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.

```
912 [~,pari]=max(nPatch+0.01*(1:2));
913 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.

```
923 switch pari
924   case 1, patches.x=codistributed(patches.x,patches.codist);
925   case 2, patches.y=codistributed(patches.y,patches.codist);
926 otherwise
927   error('should never have bad index for parallel distribution')
928 end%switch
929 end%spmd
```

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

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

Fin

```
948 end% function
```

⁶If subsequently outside `spmd`, then one must use functions like `getfield(patches{1}, 'a')`.

4.2 patchSys2(): interface 2D space to time integrators

To simulate in time with 2D spatial patches we often need to interface a users time derivative function with time integration routines such as `ode23` or `PIRK2`. This function provides an interface. Communicate patch-design variables (Section 4.1) either via the global struct `patches` or via an optional third argument. `patches` is required for the parallel computing of `spmd`, or if parameters are to be passed though to the user microscale function.

```
23 function dudt = patchSys2(t,u,patches,varargin)
24 if nargin<3, 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 `nSubP(1) × nSubP(2) × nPatch(1) × 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,patches,...)` that computes the time derivatives on the patchy lattice. The array `u` has size `nSubP(1) × nSubP(2) × nVars × nEnsem × 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) × 1 × 1 × 1 × nPatch(1) × 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 × nSubP(2) × 1 × 1 × 1 × 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.
- `varargin`, optional, is arbitrary list of parameters to be passed onto the users time-derivative function as specified in `configPatches2`.

Output

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

Reshape the fields `u` as a 6D-array, and sets the edge values from macroscale interpolation of centre-patch values. Section 4.3 describes `patchEdgeInt2()`.

```
93 sizeu = size(u);
94 u = patchEdgeInt2(u,patches);
```

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.

```
104 dudt = patches.fun(t,u,patches,varargin{:});  
105 m = patches.nEdge(1);  
106 dudt([1:m end-m+1:end],:,:) = 0;  
107 m = patches.nEdge(2);  
108 dudt(:,[1:m end-m+1:end],:) = 0;  
109 dudt = reshape(dudt,sizeu);
```

Fin.

4.3 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 et al. 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 et al. 2020](#)). This function is primarily used by patchSys2() but is also useful for user graphics.⁷

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

```
29 function u = patchEdgeInt2(u,patches)
30 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 · 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 `nSubP1×1×1×1×nPatch1×1` 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 $\{0, 2, 4, \dots\}$
 - `.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

⁷ Script `patchEdgeInt2test.m` verifies this code.

preserves symmetry); false, from centre cross-patch values (near original scheme).

- `.nEdge`, two elements, the width of edge values set by interpolation at the x, y -edge regions, respectively, of each patch (default is one for both x, y -edges).
- `.nEnsem` the number of realisations in the ensemble.
- `.parallel` whether serial or parallel.

Output

- `u` is 6D array, $n_{SubP1} \cdot n_{SubP2} \cdot n_{Vars} \cdot n_{Ensem} \cdot n_{Patch1} \cdot n_{Patch2}$, 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.

```
122     if max(abs(imag(u(:))))<1e-9*max(abs(u(:)))
123         uclean=@(u) real(u);
124     else uclean=@(u) u;
125     end
```

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

```
133 [~,ny,~,~,~,Ny] = size(patches.y);
134 [nx,~,~,~,Nx,~] = size(patches.x);
135 nEnsem = patches.nEnsem;
136 nVars = round(numel(u)/numel(patches.x)/numel(patches.y)/nEnsem);
137 assert(numel(u) == nx*ny*Nx*Ny*nVars*nEnsem ...
138 , 'patchEdgeInt2: input u has wrong size for parameters')
139 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.

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

Implement multiple width edges by folding Subsample x, y coordinates, noting it is only differences that count *and* the microgrid x, y spacing must be uniform.

```
160 %x = patches.x;
161 %if patches.nEdge(1)>1
162 % m = patches.nEdge(1);
163 % x = x(1:m:nx,:,:,:,:,:);
164 % nx = nx/m;
165 % u = reshape(u,m,nx,ny,nVars,nEnsem,Nx,Ny);
166 % nVars = nVars*m;
```

```

167  % u = reshape( permute(u,[2:3 1 4:7]) ...
168  % ,nx,ny,nVars,nEnsem,Nx,Ny);
169  %end%if patches.nEdge(1)
170  %y = patches.y;
171  %if patches.nEdge(2)>1
172  % m = patches.nEdge(2);
173  % y = y(:,1:m:ny,:,:,:);
174  % ny = ny/m;
175  % u = reshape(u,nx,m,ny,nVars,nEnsem,Nx,Ny);
176  % nVars = nVars*m;
177  % u = reshape( permute(u,[1 3 2 4:7]) ...
178  % ,nx,ny,nVars,nEnsem,Nx,Ny);
179  %end%if patches.nEdge(2)
180  x = patches.x;
181  y = patches.y;
182  if mean(patches.nEdge)>1
183    mx = patches.nEdge(1);
184    my = patches.nEdge(2);
185    x = x(1:mx:nx,:,:,:,:,:);
186    y = y(:,1:my:ny,:,:,:,:,:);
187    nx = nx/mx;
188    ny = ny/my;
189    u = reshape(u,mx,nx,my,ny,nVars,nEnsem,Nx,Ny);
190    nVars = nVars*mx*my;
191    u = reshape( permute(u,[2 4 1 3 5:8]) ...
192      ,nx,ny,nVars,nEnsem,Nx,Ny);
193  end%if patches.nEdge

```

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

```

201  i0 = round((nx+1)/2);
202  j0 = round((ny+1)/2);

```

4.3.1 Periodic macroscale interpolation schemes

```
211  if patches.periodic
```

Get the size ratios of the patches.

```

217  rx = patches.ratio(1);
218  ry = patches.ratio(2);

```

4.3.1.1 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.

```

230  ordCC = patches.ordCC;
231  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.

```

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

```

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

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

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

```

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

```

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

```

277 if patches.stag % use only odd numbered neighbours
278   error('polynomial interpolation not yet for staggered patch coupling')
279 %   dmux(:,:,(:,:,I,:,:,1) = (Ux(:,:,(:,:,Ip,:)+Ux(:,:,(:,:,Im,:))/2; % \mu
280 %   dmux(:,:,(:,:,I,:,:,2) = (Ux(:,:,(:,:,Ip,:)-Ux(:,:,(:,:,Im,:)); % \delta
281 %   Ip = Ip(Ip); Im = Im(Im); % increase shifts to \pm2
282 %   dmuy(:,:,(:,:,J,1) = (Ux(:,:,(:,:,Jp)+Ux(:,:,(:,:,Jm))/2; % \mu
283 %   dmuy(:,:,(:,:,J,2) = (Ux(:,:,(:,:,Jp)-Ux(:,:,(:,:,Jm)); % \delta
284 %   Jp = Jp(Jp); Jm = Jm(Jm); % increase shifts to \pm2
285 else %disp('starting standard interpolation')
286   dmu(:,:,(:,:,I,:,:,1) = (U(:,:,(:,:,Ip,:)
287                           -U(:,:,(:,:,Im,:))/2; %\mu\delta
288   dmu(:,:,(:,:,I,:,:,2) = (U(:,:,(:,:,Ip,:)
289                           -2*U(:,:,(:,:,I,:))+U(:,:,(:,:,Im,:)); %\delta^2
290 end% if patches.stag

```

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

```

297 for k = 3:ordCC
298   dmu(:,:,(:,:,I,:,:,k) =      dmu(:,:,(:,:,Ip,:,:,k-2) ...
299             -2*dmu(:,:,(:,:,I,:,:,k-2) +dmu(:,:,(:,:,Im,:,:,k-2));
300 end

```

Interpolate macro-values to be Dirichlet edge values for each patch ([Roberts & Kevrekidis 2007](#), [Bunder et al. 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`.

```
315 k=1+patches.EdgyInt; % use centre or two edges
316 u(nx,2:(ny-1),:,patches.ri,I,:)
317 = U(1,:,:,:, :, :)*(1-patches.stag) ...
318 +sum( shiftdim(patches.Cwtsr(:,1),-6).*dmu(1,:,:,:, :, :),7);
319 u(1,2:(ny-1),:,patches.le,I,:,:) ...
320 = U(k,:,:,:, :, :)*(1-patches.stag) ...
321 +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.

```
331 if patches.EdgyInt % interpolate next-to-face values
332 U = u(:,[2 ny-1],:,:,I,J);
333 else % interpolate centre-cross values
334 U = u(:,j0,:,:,:,I,J);
335 end;%if patches.EdgyInt
```

Adjoin extra dimension for the array of differences.

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

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

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

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

```
356 if patches.stag % use only odd numbered neighbours
357 error('polynomial interpolation not yet for staggered patch coupling')
358 else %disp('starting standard interpolation')
359 dmu(:,:, :, :, :, J,1) = (U(:,:, :, :, :, Jp) ...
360 -U(:,:, :, :, :, Jm))/2; \%mu\delta
361 dmu(:,:, :, :, :, J,2) = (U(:,:, :, :, :, Jp) ...
362 -2*U(:,:, :, :, :, J) +U(:,:, :, :, :, Jm)); \%delta^2
363 end% if stag
```

Recursively take δ^2 .

```
369 for k = 3:ordCC
370 dmu(:,:, :, :, :, J,k) = dmu(:,:, :, :, :, Jp,k-2) ...
371 -2*dmu(:,:, :, :, :, J,k-2) +dmu(:,:, :, :, :, Jm,k-2);
372 end
```

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

```

380 k = 1+patches.EdgyInt; % use centre or two edges
381 u(:,ny,:,:patches.to,:,:J) ...
382 = U(:,1,:,:,:,:)*(1-patches.stag) ...
383 +sum( shiftdim(patches.Cwtsr(:,2),-6).*dmu(:,1,:,:,:,:,:) ,7);
384 u(:,1 ,:,patches.bo,:,:J) ...
385 = U(:,k,:,:,:,:)*(1-patches.stag) ...
386 +sum( shiftdim(patches.Cwtsl(:,2),-6).*dmu(:,k,:,:,:,:,:) ,7);

```

4.3.1.2 Case of spectral interpolation

Assumes the domain is macro-periodic.

```
397 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 $\mathbf{ks} = k2\pi/N$ for ‘wavenumbers’ $k = (0, 1, \dots, k_{\max}, -k_{\max}, \dots, -1)$ for odd N , and $k = (0, 1, \dots, k_{\max}, \pm(k_{\max} + 1) - k_{\max}, \dots, -1)$ 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.

```

420 if patches.stag % transform by doubling the number of fields
421 error('staggered grid not yet implemented??')
422 v=nan(size(u)); % currently to restore the shape of u
423 u=cat(3,u(:,1:2:nPatch,:),u(:,2:2:nPatch,:));
424 stagShift=reshape(0.5*[ones(nVars,1);-ones(nVars,1)],1,1,[]);
425 iV=[nVars+1:2*nVars 1:nVars]; % scatter interp to alternate field
426 r=r/2; % ratio effectively halved
427 nPatch=nPatch/2; % halve the number of patches
428 nVars=nVars*2; % double the number of fields
429 else % the values for standard spectral
430     stagShift = 0;
431     iV = 1:nVars;
432 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.

```
442 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, $k = (0, 1, \dots, k_{\max}, +k_{\max} + 1) - k_{\max}, \dots, -1)$.

```
455     kMax = floor((Nx-1)/2);
456     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`.

```
469 if ~patches.EdgyInt
470     Cm = fft( u(i0, iy, :, :, :, :) , [] , 5 );
471     Cp = Cm;
472 else
473     Cm = fft( u( 2, iy , :, patches.le, :, :) , [] , 5 );
474     Cp = fft( u(nx-1, iy , :, patches.ri, :, :) , [] , 5 );
475 end%if ~patches.EdgyInt
```

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

```
482 u(nx, iy, :, :, :, :) = uclean( ifft( ...
483     Cm.*exp(1i*(stagShift+kr)) , [] , 5 ) );
484 u( 1, iy, :, :, :, :) = uclean( ifft( ...
485     Cp.*exp(1i*(stagShift-kr)) , [] , 5 ) );
```

y-normal edge values Set wavenumbers into a vector.

```
495     kMax = floor((Ny-1)/2);
496     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.

```
503 if ~patches.EdgyInt
504     Cm = fft( u(:, j0, :, :, :, :) , [] , 6 );
505     Cp = Cm;
506 else
507     Cm = fft( u(:, 2 , :, patches.bo, :, :) , [] , 6 );
508     Cp = fft( u(:, ny-1 , :, patches.to, :, :) , [] , 6 );
509 end%if ~patches.EdgyInt
```

Invert the Fourier transforms to complete interpolation.

```
515 u(:, ny, :, :, :, :) = uclean( ifft( ...
516     Cm.*exp(1i*(stagShift+kr)) , [] , 6 ) );
517 u(:, 1, :, :, :, :) = uclean( ifft( ...
518     Cp.*exp(1i*(stagShift-kr)) , [] , 6 ) );
524 end% if ordCC>0 else, so spectral
```

4.3.2 Non-periodic macroscale interpolation

```

535 else% patches.periodic false
536 assert(~patches.stag, ...
537 '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.

```

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

```

4.3.2.1 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.⁸

```

569 F = nan(patches.EdgyInt+1,ny-2,nVars,nEnsem,Nx,Ny,px+1);
570 if patches.EdgyInt % interpolate next-to-edge values
571     F(:,:,:,:,1,:)=u([nx-1 2],iy,:,:,:,:,:);
572     X = x([nx-1 2],:,:,:,:,:,:);
573 else % interpolate mid-patch cross-patch values
574     F(:,:,:,:,1,:)=u(i0,iy,:,:,:,:,:);
575     X = x(i0,:,:,:,:,:,:,:);
576 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.

```

587 for q = 1:px
588     i = 1:Nx-q;
589     F(:,:,:,:,i,:q+1) ...
590     = (F(:,:,:,:,i+1 ,:,q)-F(:,:,:,:,i,:,q)) ...
591     ./ (X(:,:,:,:,i+q,:)-X(:,:,:,:,i,:));
592 end

```

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

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

⁸ **ToDo:** Have no plans to implement core averaging as yet.

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.

```

612     i = max(1,min(1:Nx,Nx-ceil(px/2))-floor(px/2));
613     Uedge = F(:,:, :, :, i, :, px+1);
614     for q = px:-1:1
615         Uedge = F(:,:, :, :, i, :, q)+(Xedge-X(:,:, :, :, i+q-1,:)).*Uedge;
616     end

```

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

```

624     u(1 ,iy,:,:patches.le,:,:)= Uedge(1,:,:,:, :, :);
625     u(nx, iy,:,:patches.ri,:,:)= Uedge(2,:,:,:, :, :);

```

4.3.2.2 y -direction values

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

```

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

```

Form tables of divided differences.

```

647     for q = 1:py
648         j = 1:Ny-q;
649         F(:,:, :, :, :, j, q+1) ...
650             = (F(:,:, :, :, :, j+1 ,q)-F(:,:, :, :, :, j, q)) ...
651             ./ (Y(:,:, :, :, :, j+q) -Y(:,:, :, :, :, j));
652     end

```

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

```

659     Yedge = 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.

```

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

```

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

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

4.3.2.3 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, unless testing, override their computed interpolation values with NaN.

```
692 if isfield(patches,'intTest')&&patches.intTest
693 else % usual case
694     u( 1,:,:,:, 1,:) = nan;
695     u(nx,:,:,:,Nx,:) = nan;
696     u(:, 1,:,:,:, 1) = nan;
697     u(:,ny,:,:,:,Ny) = nan;
698 end%if
```

End of the non-periodic interpolation code.

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

Unfold multiple edges No need to restore x, y .

```
712 if mean(patches.nEdge)>1
713     nVars = nVars/(mx*my);
714     u = reshape( u ,nx,ny,mx,my,nVars,nEnsem,Nx,Ny);
715     nx = nx*mx;
716     ny = ny*my;
717     u = reshape( permute(u,[3 1 4 2 5:8]) ...
718                 ,nx,ny,nVars,nEnsem,Nx,Ny);
719 end%if patches.nEdge
```

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

```
727 end% function patchEdgeInt2
```

4.4 wave2D: example of a wave on patches in 2D

Section contents

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For $u(x, y, t)$, test and simulate the simple wave PDE in 2D space:

$$\frac{\partial^2 u}{\partial t^2} = \nabla^2 u.$$

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

1. configPatches2
2. ode15s integrator \mapsto patchSys2 \mapsto wavePDE
3. process results

Establish the global data struct `patches` to interface with a function coding the wave PDE: to be solved on 2π -periodic domain, with 9×9 patches, spectral interpolation (0) couples the patches, each patch of half-size ratio 0.25 (big enough for visualisation), and with a 5×5 micro-grid within each patch.

```
35 global patches
36 nSubP = 5;
37 nPatch = 9;
38 configPatches2(@wavePDE, [-pi pi], nan, nPatch, 0, 0.25, nSubP);
```

4.4.1 Check on the linear stability of the wave PDE

Construct the systems Jacobian via numerical differentiation. Set a zero equilibrium as basis. Then find the indices of patch-interior points as the only ones to vary in order to construct the Jacobian.

```
51 disp('Check linear stability of the wave scheme')
52 uv0 = zeros(nSubP,nSubP,2,1,nPatch,nPatch);
53 uv0([1 end],:,:,:,:,:) = nan;
54 uv0(:,[1 end],:,:,:,:,:) = nan;
55 i = find(~isnan(uv0));
```

Now construct the Jacobian. Since this is a *linear* wave PDE, use large perturbations.

```
62 small = 1;
63 jac = nan(length(i));
64 sizeJacobian = size(jac)
65 for j = 1:length(i)
66     uv = uv0(:);
67     uv(i(j)) = uv(i(j))+small;
```

```

68     tmp = patchSys2(0,uv)/small;
69     jac(:,j) = tmp(i);
70 end

```

Now explore the eigenvalues a little: find the ten with the biggest real-part; if these are small enough, then the method may be good.

```

78 evals = eig(jac);
79 nEvals = length(evals)
80 [~,k] = sort(-abs(real(evals)));
81 evalsWithBiggestRealPart = evals(k(1:10))
82 if abs(real(evals(k(1))))>1e-4
83     warning('eigenvalue failure: real-part > 1e-4')
84     return, end

```

Check that the eigenvalues are close to true waves of the PDE (not yet the micro-discretised equations).

```

91 kwave = 0:(nPatch-1)/2;
92 freq = sort(reshape(sqrt(kwave.^2+kwave.^2),1,[]));
93 freq = freq(diff([-1 freq])>1e-9);
94 freqerr = [freq; min(abs(imag(evals)-freq))]

```

4.4.2 Execute a simulation

Set a Gaussian initial condition using auto-replication of the spatial grid: here u_0 and v_0 are in the form required for computation: $n_x \times n_y \times 1 \times 1 \times N_x \times N_y$.

```

109 u0 = exp(-patches.x.^2-patches.y.^2);
110 v0 = zeros(size(u0));

```

Initiate a plot of the simulation using only the microscale values interior to the patches: set x and y -edges to `nan` to leave the gaps. Start by showing the initial conditions of [Figure 4.1](#) while the simulation computes. To mesh/surf plot we need to ?? ‘transpose’ to size $n_x \times N_x \times n_y \times N_y$, then reshape to size $n_x \cdot N_x \times n_y \cdot N_y$.

```

122 x = squeeze(patches.x); y = squeeze(patches.y);
123 x([1 end],:) = nan; y([1 end],:) = nan;
124 u = reshape(permute(squeeze(u0),[1 3 2 4]), [numel(x) numel(y)]);
125 usurf = surf(x(:,y(:,u')));
126 axis([-3 3 -3 3 -0.5 1]), view(60,40)
127 xlabel('space $x$'), ylabel('space $y$'), zlabel('$u(x,y)$')
128 legend('time = 0','Location','north')
129 colormap(hsv)
130 drawnow
131 ifOursCf2eps([mfilename 'ic'])

```

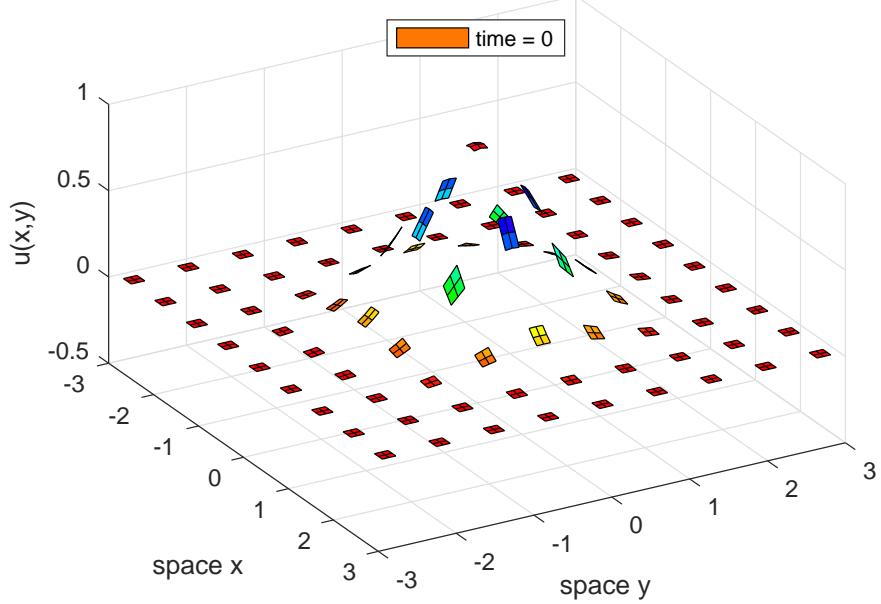
Integrate in time using standard functions.

```

144 disp('Wait while we simulate u_t=v, v_t=u_xx+u_yy')
145 uv0 = cat(3,u0,v0);
146 if ~exist('OCTAVE_VERSION','builtin')

```

Figure 4.3: initial field $u(x, y, t)$ at time $t = 0$ of the patch scheme applied to the simple wave PDE: [Figure 4.4](#) plots the computed field at time $t = 2$.



```

147 [ts,uv0] = ode23( @patchSys2,[0 6],uv0(:));
148 else % octave version is slower
149 [ts,uv0] = odeOcts(@patchSys2,linspace(0,6),uv0(:));
150 end

```

Animate the computed simulation to end with [Figure 4.4](#). Because of the very small time-steps, subsample to plot at most 100 times.

```

158 di = ceil(length(ts)/100);
159 for i = [1:di:length(ts)-1 length(ts)]
160   uv = patchEdgeInt2(uvs(i,:));
161   uv = reshape(permute(uv,[1 5 2 6 3 4]), [numel(x) numel(y) 2]);
162   set(usrurf,'ZData', uv(:,:,1));
163   legend(['time = ', num2str(ts(i),2)])
164   pause(0.1)
165 end
166 if0urCf2eps([mfilename 't' num2str(ts(end))])

```

4.4.3 wavePDE(): Example of simple wave PDE inside patches

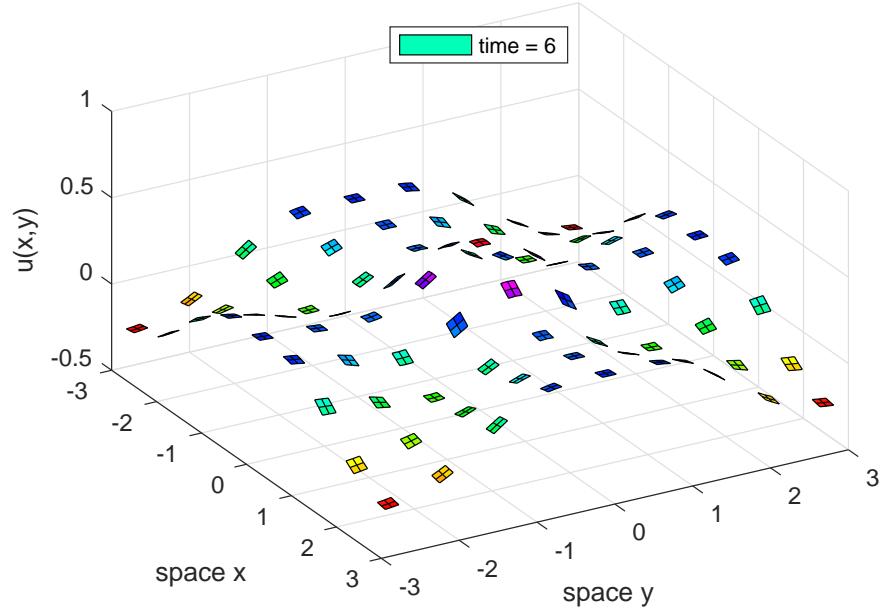
As a microscale discretisation of $u_{tt} = \nabla^2(u)$, so code $\dot{u}_{ijkl} = v_{ijkl}$ and $\ddot{v}_{ijkl} = \frac{1}{\delta x^2}(u_{i+1,j,k,l} - 2u_{i,j,k,l} + u_{i-1,j,k,l}) + \frac{1}{\delta y^2}(u_{i,j+1,k,l} - 2u_{i,j,k,l} + u_{i,j-1,k,l})$.

```

14 function uvt = wavePDE(t,uv,patches)
15   dx = diff(patches.x(1:2));
16   dy = diff(patches.y(1:2)); % microscale spacing
17   i = 2:size(uv,1)-1;
18   j = 2:size(uv,2)-1; % interior patch-points
19   uvt = nan+uv; % preallocate storage
20   uvt(i,j,1,:) = uv(i,j,2,:);

```

Figure 4.4: field $u(x, y, t)$ at time $t = 6$ of the patch scheme applied to the simple wave PDE with initial condition in Figure 4.3.



```

21     uvt(i,j,2,:) = diff(uv(:,j,1,:),2,1)/dx^2 ...
22             +diff(uv(i,:,:1,:),2,2)/dy^2;
23 end

10 function [ts,xs] = ode0cts(dxdt,tSpan,x0)
11     if length(tSpan)>2, ts = tSpan;
12     else ts = linspace(tSpan(1),tSpan(end),21)';
13     end
14     lsode_options('integration method','non-stiff');
15     xs = lsode(@(x,t) dxdt(t,x),x0,ts);
16 end

```

4.5 homoDiffEdgy2: computational homogenisation of a 2D diffusion via simulation on small patches

This section extends to 2D the 1D code discussed in [Section 3.5](#). First set random heterogeneous diffusivities of random period in each of the two directions. Crudely normalise by the harmonic mean so the decay time scale is roughly one.

```
23 mPeriod = randi([2 3],1,2)
24 cHetr = exp(1*randn([mPeriod 2]));
25 cHetr = cHetr*mean(1./cHetr(:))
```

Configure the patch scheme with some arbitrary choices of domain, patches, size ratios. Use spectral interpolation as we test other orders subsequently. In 2D we appear to get only real eigenvalues by using edgy interpolation. What happens for non-edgy interpolation is unknown.

```
36 edgyInt = true;
37 nEnsem = 1 %prod(mPeriod) % or just set one
38 if nEnsem==1% use more patches
39     nPatch = [9 9]
40     nSubP = (2-edgyInt)*mPeriod+1+edgyInt
41 else % when nEnsem>1 use fewer patches
42     nPatch = [5 5]
43     nSubP = mPeriod+randi([1 4],1,2) % +2 is decoupled
44 end
45 ratio = 0.2+0.2*rand(1,2)
46 configPatches2(@heteroDiff2,[-pi pi -pi pi],nan,nPatch ...
47 ,0, ratio, nSubP , 'EdgyInt',edgyInt , 'nEnsem',nEnsem ...
48 , 'hetCoeffs',cHetr );
```

Simulate Set initial conditions of a simulation, replicated for each in the ensemble.

```
58 global patches
59 u0 = 0.8*cos(patches.x).*sin(patches.y) ...
60     +0.1*randn([nSubP,1,1,nPatch]);
61 u0 = repmat(u0,1,1,1,nEnsem,1,1);
```

Integrate using standard integrators, unevenly spaced in time to better display transients.

```
68 if ~exist('OCTAVE_VERSION','builtin')
69     [ts,us] = ode23(@patchSys2, 0.3*linspace(0,1).^2, u0(:));
70 else % octave version
71     [ts,us] = ode0cts(@patchSys2, 0.3*linspace(0,1).^2, u0(:));
72 end
```

Plot the solution as an animation over time.

```
79 if ts(end)>0.099, disp('plot animation of solution field')
80 figure(1), clf, colormap(hsv)
```

Get spatial coordinates and pad them with NaNs to separate patches.

```
87 x = squeeze(patches.x); y = squeeze(patches.y);
88 x(end+1,:)=nan; y(end+1,:)=nan; % pad with nans
```

For every time step draw the surface and pause for a short display.

```
95 for i = 1:length(ts)
```

Get the row vector of data, form into the 6D array via the interpolation to the edges, then pad with Nans between patches, and reshape to suit the surf function.

```
103 u = squeeze( mean(patchEdgeInt2(us(i,:),),4));
104 u(end+1,:,:,:)=nan; u(:,end+1,:,:)=nan;
105 u = reshape(permute(u,[1 3 2 4]), [numel(x) numel(y)]);
```

If the initial time then draw the surface with labels, otherwise just update the surface data.

```
112 if i==1
113     hsurf = surf(x(:,y(:,u')); view(60,40)
114     axis([-pi pi -pi pi -1 1]), caxis([-1 1])
115     xlabel('$x$'), ylabel('$y$'), zlabel('$u(x,y)$')
116 else set(hsurf,'ZData', u');
117 end
118 legend(['time = ' num2str(ts(i),2)],'Location','north')
119 pause(0.05)
```

finish the animation loop and if-plot.

```
125 end%for over time
126 end%if-plot
```

4.5.1 Compute Jacobian and its spectrum

Let's explore the Jacobian dynamics for a range of orders of interpolation, all for the same patch design and heterogeneity. Except here use a small ratio as we do not plot.

```
142 ratio = [0.1 0.1]
143 nLeadEvals=prod(nPatch)+max(nPatch);
144 leadingEvals=[];
```

Evaluate eigenvalues for spectral as the base case for polynomial interpolation of order 2, 4,

```
152 maxords=10;
153 for ord=0:2:maxords
    ord=ord
```

Configure with same parameters, then because they are reset by this configuration, restore coupling.

```

161 configPatches2(@heteroDiff2,[-pi pi -pi pi],nan,nPatch ...
162 ,ord, ratio, nSubP, 'EdgyInt', edgyInt, 'nEnsem', nEnsem ...
163 , 'hetCoeffs', cHetr);

```

Find which elements of the 6D array are interior micro-grid points and hence correspond to dynamical variables.

```

170 u0 = zeros([nSubP,1,nEnsem,nPatch]);
171 u0([1 end],:,:) = nan;
172 u0(:,[1 end],:) = nan;
173 i = find(~isnan(u0));

```

Construct the Jacobian of the scheme as the matrix of the linear transformation, obtained by transforming the standard unit vectors.

```

181 jac = nan(length(i));
182 sizeJacobian = size(jac)
183 for j = 1:length(i)
184     u = u0(:)+(i(j)==(1:numel(u0))');
185     tmp = patchSys2(0,u);
186     jac(:,j) = tmp(i);
187 end

```

Test for symmetry, with error if we know it should be symmetric.

```

194 notSymmetric=norm(jac-jac')
195 if edgyInt, assert(notSymmetric<1e-7,'failed symmetry')
196 elseif notSymmetric>1e-7, disp('failed symmetry')
197 end

```

Find all the eigenvalues (as `eigs` is unreliable).

```

203 if edgyInt, [evecs,evals] = eig((jac+jac')/2,'vector');
204 else evals = eig(jac);
205 end
206 biggestImag=max(abs(imag(evals)));
207 if biggestImag>0, biggestImag=biggestImag, end

```

Sort eigenvalues on their real-part with most positive first, and most negative last. Store the leading eigenvalues in `egs`, and write out when computed all orders. The number of zero eigenvalues, `nZeroEv`, gives the number of decoupled systems in this patch configuration.

```

217 [~,k] = sort(-real(evals));
218 evals=evals(k); evecs=evecs(:,k);
219 if ord==0, nZeroEv=sum(abs(evals(:))<1e-5), end
220 if ord==0, evec0=evecs(:,1:nZeroEv*nLeadEvals);
221 else % find evec closest to that of each leading spectral
222     [~,k]=max(abs(evecs'*evec0));
223     evals=evals(k); % sort in corresponding order
224 end
225 leadingEvals=[leadingEvals evals(nZeroEv*(1:nLeadEvals))];
226 end

```

```

227 disp('      spectral      quadratic      quartic      sixth-order ...')
228 leadingEvals=leadingEvals

Plot the errors in the eigenvalues using the spectral ones as accurate. Only
plot every second, iEv, as all are repeated eigenvalues.

237 if maxords>2
238     iEv=2:2:12;
239     figure(2);
240     err=abs(leadingEvals-leadingEvals(:,1)) ...
241         ./(1e-7+abs(leadingEvals(:,1)));
242     semilogy(2:2:maxords,err(iEv,2:end)', 'o:');
243     xlabel('coupling order')
244     ylabel('eigenvalue relative error')
245     leg=legend( ...
246         strcat('$',num2str(real(leadingEvals(iEv,1)), '%.4f'), '$') ...
247         , 'Location', 'northeastoutside');
248     if ~exist('OCTAVE_VERSION','builtin')
249         title(leg,'eigenvalues'), end
250     legend boxoff
251 end%if-plot

```

4.5.2 heteroDiff2(): heterogeneous diffusion

This function codes the lattice heterogeneous diffusion inside the patches. For 6D input arrays u , x , and y (via edge-value interpolation of `patchSys2`, [Section 4.2](#)), computes the time derivative (3.1) at each point in the interior of a patch, output in ut . The two 2D array of diffusivities, c_{ij}^x and c_{ij}^y , have previously been stored in `patches.cs` (3D).

```

19 function ut = heteroDiff2(t,u,patches)
20     dx = diff(patches.x(2:3)); % x space step
21     dy = diff(patches.y(2:3)); % y space step
22     ix = 2:size(u,1)-1; % x interior points in a patch
23     iy = 2:size(u,2)-1; % y interior points in a patch
24     ut = nan+u;           % preallocate output array
25     ut(ix,iy,:,:,:,:,:) ...
26     = diff(patches.cs(:,iy,1,:).*diff(u(:,iy,:,:,:,:),1,1)/dx^2 ...
27         +diff(patches.cs(ix,:,2,:).*diff(u(ix,:,:,:,:,:),1,2),1,2)/dy^2;
28 end% function

```

Fin.

4.6 homoDiffSoln2: steady state of a 2D heterogeneous diffusion via small patches

Here we find the steady state $u(x, y)$ to the heterogeneous PDE

$$u_t = \vec{\nabla} \cdot [c(x, y) \vec{\nabla} u] - u + f, \quad \text{for } f = 100 \sin(\pi x) \sin(\pi y).$$

The heterogeneous diffusion c varies over two orders of magnitude in small space distance ϵ . I include $-u$ in the PDE to ensure a steady state with periodic BCs.

[Section 4.6.2](#) gives a function that we invoke to explore the errors in the patch scheme solution. The spectral patch scheme is essentially exact.

[Biezemans et al. \(2022\)](#) discussed an example homogenisation in 2D with heterogeneity of period $\epsilon := \pi/150$ in both directions. Ensure integer multiple of heterogeneity periods in the domain, and initially use three times bigger ϵ .

```
35 epsilon = 1/round(50/pi)
```

[Biezemans et al. \(2022\)](#) choose microscale mesh spacing of $1/1024$, so the number of micro-grid points in one period would be 1024ϵ . But *initially* use less.

```
44 mPeriod = round(128*epsilon) %round(1024*epsilon)
```

So the migro-grid spacing is exactly

```
50 dx = epsilon/mPeriod
```

Diffusivities Now form one period of the heterogeneity diffusivities. [Biezemans et al. \(2022\)](#) used $c = 1 + 100 \cos^2(\pi x/\epsilon) \sin^2(\pi y/\epsilon)$. Need to shift phases of the diffusivity by half-micro-grid for diffusivities in each direction to form two diffusivity matrices on the microscale lattice. Variables h, v represent $\pi x/\epsilon$ or $\pi y/\epsilon$.

```
64 cHetr=[];
65 v=pi*( 1:mPeriod)/mPeriod;
66 h=pi*(0.5:mPeriod)/mPeriod;
67 cHetr(:,:,1) = 1+100*cos(h').^2*sin(v).^2;
68 cHetr(:,:,2) = 1+100*cos(v').^2*sin(h).^2;
```

Plot surfaces of the diffusivity.

```
74 figure(2),surf(h/pi,v/pi,cHetr(:,:,2))
75 hold on, surf(v/pi,h/pi,cHetr(:,:,1))
76 hold off, alpha 0.5, drawnow
```

Patch configuration As is common, [Biezemans et al. \(2022\)](#) implemented zero-Dirichlet BCs on $(0, 1)^2$. Here these are more-or-less encompassed by implementing periodic BCs on $(-1, 1)^2$. Initially use 8×8 patches to have 4×4 patches in $(0, 1)^2$, which then have patch spacing H .

```

89 nPatch = [8 8]
90 H = 2./nPatch
91 HepsilonRatio = H/epsilon

```

Best when each patch spans an integral number of periods plus one grid step.
The smallest such patches are

```

98 nSubP = [1 1]*mPeriod+2

```

Consequently, the ratio of space computed on, to the space in the domain is the product of the following ratios in each direction, namely about 8% here.

```

106 ratio = ((nSubP-2)*dx)./H

```

Specify spectral interpolation. The edgy interpolation is self-adjoint ([Bunder et al. 2020](#)) leading to a symmetric matrix problem.

```

114 configPatches2(@hetDiffForce2, [-1 1 -1 1], nan, nPatch ...
115 , 0, ratio, nSubP, 'EdgyInt', true ...
116 , 'hetCoeffs', cHetr );

```

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.

```

128 global patches i
129 u0 = zeros([nSubP,1,1,nPatch]);
130 u0([1 end],:,:) = nan; u0(:,[1 end],:) = nan;
131 i = find(~isnan(u0));
132 nVars = numel(i)

```

Solve by iteration. Could use `fsolve` for nonlinear problems, but for linear it is much faster to use Conjugate-Gradient algorithm. `gmres` is competitive, but appears to take twice as long.

```

142 tic;
143 if 0, uSoln=fsolve(@theRes,u0(i));

```

The above is for nonlinear PDEs. For linear PDEs, determine the RHS vector, and make a function that computes the matrix vector product.

```

151 else
152     maxIt = ceil(nVars/10);
153     rhsb = theRes(u0(i));
154     uSoln = pcg(@(u) rhsb-theRes(u),rhsb,1e-9,maxIt);
155 end
156 solnTime = toc

```

Store the solution into the patches, and give magnitudes.

```

162 u0(i) = uSoln;
163 normSoln = norm(uSoln)
164 normResidual = norm(theRes(uSoln))

```

Draw solution profile First reshape arrays to suit 2D space surface plots.

```

172 figure(1), clf, colormap(hsv)
173 x = squeeze(patches.x); y = squeeze(patches.y);
174 u = reshape(permute(squeeze(u0),[1 3 2 4]), [numel(x) numel(y)]);

```

Draw the patch solution surface in the positive quadrant, with edge-values omitted as already NaN by not bothering to interpolate them.

```

182 surf(x(:,y(:,u')); view(60,40)
183 maxu = ceil(max(u(:))*10)/10;
184 axis([0 1 0 1 0 maxu]), caxis([0 maxu])
185 xlabel('$x$'), ylabel('$y$'), zlabel('$u(x,y)$')

```

Assess errors in the patch scheme Invoke the function with desired interpolation: 0, spectral; 2, 4, ..., polynomial.

```
194 errorsPatchScheme(0)
```

4.6.1 Microscale discretisation inside patches

hetDiffForce2(): heterogeneous diffusion PDE This function, based upon [Section 4.5.2](#), 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 . The two 2D array of diffusivities, c_{ij}^x and c_{ij}^y , are stored in `patches.cs` (3D).

```

213 function ut = hetDiffForce2(t,u,patches)
214     dx = diff(patches.x(2:3)); % x space step
215     dy = diff(patches.y(2:3)); % y space step
216     ix = 2:size(u,1)-1; % x interior points in a patch
217     iy = 2:size(u,2)-1; % y interior points in a patch
218     ut = nan+u;           % preallocate output array
219     fu = -u+100*sin(pi*patches.x).*sin(pi*patches.y);
220     ut(ix,iy,:,:,:, :) ...
221     = diff(patches.cs(:,iy,1).*diff(u(:,iy,:,:,:,1),1),1)/dx^2 ...
222     +diff(patches.cs(ix,:,2).*diff(u(ix,:,:,:,1,2),1,2),1,2)/dy^2 ...
223     +fu(ix,iy,:,:,:, :);
224 end% function

```

theRes(): 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, and returns the vector of patch-interior time derivatives.

```

236 function f=theRes(u)
237 global i patches
238 v=nan(size(patches.x+patches.y));
239 v(i)=u;
240 f=patchSys2(0,v(:,),patches);
241 f=f(i);
242 end

```

4.6.2 Function to explore errors in the patch scheme

We find the spectral interpolation patch scheme accurate to essentially zero errors, namely errors less than 10^{-10} . Non-spectral interpolation has errors that decrease roughly like expected power of patch spacing.

The single argument `ord` is 0 for spectral interpolation and 2, 4, ... for corresponding polynomial interpolation schemes.

```
262 function errorsPatchScheme(ord)
263 warning('Assessing errors via varying number of patches')
```

Use a hierarchy of cases with increasing number of patches—the number increasing by 3^2 from one level to the next in the hierarchy. Then the higher resolution patches precisely contain the lower resolution cases. The case when index `k=kMax` corresponds to the full-domain solution. [Biezemans et al. \(2022\)](#) use heterogeneity of period $\epsilon := \pi/150 \approx 0.021$ in both directions, here with `kMax=3` use $\epsilon \approx 0.037$. Ensure integer multiple of heterogeneity periods in the full domain.

```
279 kMax = 3
280 epsilon = 1/3^kMax
```

[Biezemans et al. \(2022\)](#) choose microscale mesh spacing of 1/1024, so their number of micro-grid points in one period is $1024\epsilon \approx 21$. But here use less because less is plenty enough—the issue is the accuracy of the patch scheme to whatever micro-grid system is given, *not* the accuracy of the micro-grid system to the PDE.

```
292 mPeriod = 9
```

So the migro-grid spacing is

```
298 dx = epsilon/mPeriod
```

Diffusivities Now form one period of the heterogeneity diffusivities exactly as in above code.

```
307 cHetr=[];
308 v=pi*( 1:mPeriod)/mPeriod;
309 h=pi*(0.5:mPeriod)/mPeriod;
310 cHetr(:,:,1) = 1+100*cos(h').^2*sin(v).^2;
311 cHetr(:,:,2) = 1+100*cos(v').^2*sin(h).^2;
```

Loop over different patch spacings

```
319 for k=1:kMax
320 nPatch = [2 2]*3^k
```

Patch configuration Zero-Dirichlet BCs on $(0, 1)^2$ are more-or-less encompassed by implementing periodic BCs on $(-1, 1)^2$.

```
330 H = 2./nPatch
331 HepsilonRatio = H/epsilon
```

Best when each patch spans an integral number of periods plus one grid step. The smallest such patches are

```
338 nSubP = [1 1]*mPeriod+2
```

Consequently, the ratios of space computed on is the following. The case $k=kMax$ gives a ratio of precisely one that characterises a full-domain problem.

```
346 ratio = ((nSubP-2)*dx)./H
```

The edgy interpolation leads to a symmetric matrix problem (Bunder et al. 2020).

```
353 configPatches2(@hetDiffForce2, [-1 1 -1 1], nan, nPatch ...
354     , ord, ratio, nSubP, 'EdgyInt', true ...
355     , 'hetCoeffs', cHetr );
```

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.

```
367 global patches i
368 u0 = zeros([nSubP,1,1,nPatch]);
369 u0([1 end],:,:) = nan; u0(:,[1 end],:) = nan;
370 i = find(~isnan(u0));
371 nVars = numel(i)
```

For this linear problem it is fast to solve with the Conjugate-Gradient algorithm. Determine the RHS vector, and use a function that computes the matrix vector product.

```
380 tic
381 rhsb = theRes(u0(i));
382 uSoln = pcg(@(u) rhsb-theRes(u),rhsb,1e-6,999);
383 solnTime = toc
```

Store the solution into the patches, and trace magnitudes.

```
389 u0(i) = uSoln;
390 normSoln = norm(uSoln)
391 normResidual = norm(theRes(uSoln))
```

End loop over different patch spacings Store 4D field values in cell array for post-processing.

```
399 us{k}=squeeze(u0);
400 end%for
```

Compare errors across cases There are nine patches common to all grids (36 if one counts all quadrants), indexed by the following patch indices.

```
410 disp('**** Relate errors for different patch spacing ****')
411 if ord==0, disp('**** Spectral interpolation between patches')
412 else disp(['**** Polynomial interpolation, order ' num2str(ord)])
```

```

413 end
414 i=2:nSubP-1;
415 I{1}=1:3;
416 for k=2:kMax, I{k}=3*I{k-1}-1; end

```

Determine errors by computing difference between patch schemes: the final patch scheme is a full-domain solution and hence ‘exact’. Look at the RMS error in each of the patches. Find the overall error for each patch, their ratios, and the rough order of decrease.

```

426 rmsError=[]; errorRatios=[]; orderInH=[];
427 for k=1:kMax-1
428     error{k}=us{k}(i,i,I{k},I{k})-us{kMax}(i,i,I{kMax},I{kMax});
429     rmsError(:,:,k)=squeeze(rms(rms(error{k})));
430     if (k>1)&(ord>0)
431         errorRatios(:,:,k-1)=rmsError(:,:,k)./rmsError(:,:,k-1);
432         orderInH(:,:,k-1)=-log(errorRatios(:,:,k-1))/log(3);
433     end
434 end

```

Display the results, and end the function.

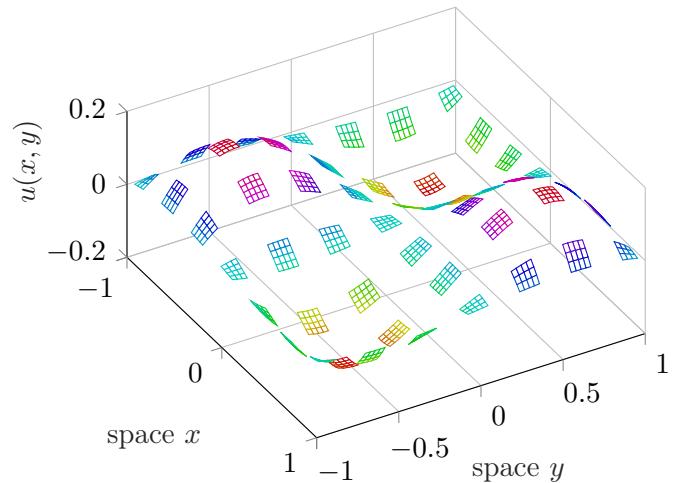
```

440 rmsError=rmsError
441 errorRatios=errorRatios
442 orderInH=orderInH
443 end%function

```

Fin.

Figure 4.5: Equilibrium of the macroscale diffusion problem of Freese with Dirichlet zero-value boundary conditions (Section 4.7). The patch size is not small so we can see the patches.



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

Here we find the steady state $u(x, y)$, see Figure 4.5, to the heterogeneous PDE (inspired by Freese et al.⁹ §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

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

and for forcing $f(x, y)$ such that the exact equilibrium is $u = x(1 - e^{1-|x|})y(1 - e^{1-|y|})$. 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.

```
57 clear all
58 global patches
59 %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.

⁹ <http://arxiv.org/abs/2211.13731>

```

70 nPatch = 7
71 nSubP = 5
72 dx = 0.03

Specify some order of interpolation.

78 configPatches2(@monoscaleDiffForce2,[-1 1 -1 1], 'equispace' ...
79 ,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 4.7.1](#).

```

87 x=patches.x; y=patches.y;
88 patches.A = sin(pi*x).*sin(pi*y);
89 patches.fu = ...
90     +2*patches.A.*((9*x.^2.*y.^2-3*x.^2-3*y.^2+1) ...
91     +12*x.*y.*((x.^2+y.^2-2));

```

By construction, the PDE has analytic solution

```
97 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.

```

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

```

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

```

121 tic;
122 uSoln = fsolve(@theRes,u0(patches.i) ...
123     ,optimoptions('fsolve','Display','off'));
124 solnTime = toc
125 normResidual = norm(theRes(uSoln))
126 normSoln = norm(uSoln)
127 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.

```

135 u0(patches.i) = uSoln;
136 u0 = patchEdgeInt2(u0);

```

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

```

147 figure(1), clf, colormap(0.8* hsv)
148 x(end+1,:,:)=nan; u0(end+1,:,:)=nan;

```

```

149 y(:,end+1,:)=nan; u0(:,end+1,:)=nan;
150 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.

157 mesh(x(:,y(:,u'));
158 xlabel('space $x$'), ylabel('space $y$'), zlabel('$u(x,y)$')
159 if0urCf2tex(mfilename)%optionally save

```

4.7.1 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 .

```

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

```

Set Dirichlet boundary value of zero around the square domain.

```

188 u( 1 ,:,:, :, 1 ,:) = 0; % left edge of left patches
189 u(end,:,:,:,end,:) = 0; % right edge of right patches
190 u(:, 1 ,:,:, :, 1 ) = 0; % bottom edge of bottom patches
191 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.

```

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

```

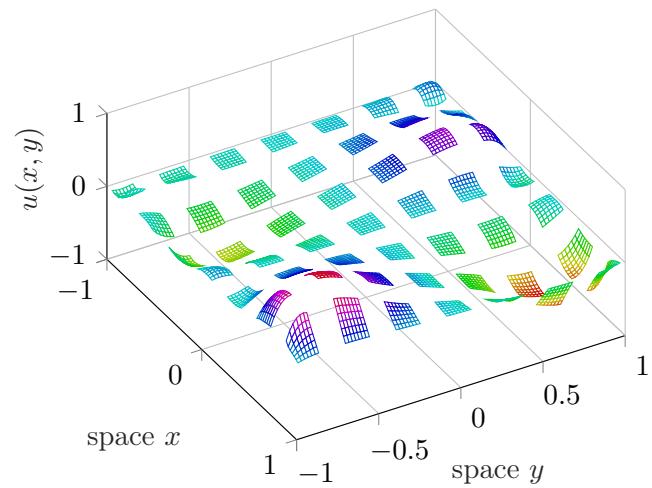
Compute the time derivatives via stored forcing and coefficients. Easier to code by conflating the last four dimensions into the one $,:$.

```

210 ut(i,j,:)
211 = 2*diff(u(:,j,:),2,1)/dx^2 +2*diff(u(i,:,:),2,2)/dy^2 ...
212 +2*patches.A(i,j,:).*( u(i+1,j+1,:)-u(i-1,j+1,:)) ...
213 -u(i+1,j-1,:)+u(i-1,j-1,:))/(4*dx*dy) ...
214 -patches.fu(i,j,:);
215 end%function monoscaleDiffForce2

```

Figure 4.6: Equilibrium of the multiscale diffusion problem of Freese with Dirichlet zero-value boundary conditions (Section 4.8). 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.



4.8 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.¹⁰ §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.

```
41 clear all
42 global patches
43 %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.

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

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

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

¹⁰ <http://arxiv.org/abs/2211.13731>

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

```
79 nPatch = 7
80 configPatches2(@twoscaleDiffForce2, [-1 1], 'equispace' ...
81 ,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 4.9.1](#).

```
89 x = patches.x; y = patches.y;
90 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.

```
104 u0 = zeros(nSubP,nSubP,1,1,nPatch,nPatch);
105 u0([1 end],:,:) = nan; u0(:,[1 end],:) = nan;
106 patches.i = find(~isnan(u0));
107 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 3.19](#)), and give magnitudes.

```
116 tic;
117 uSoln = fsolve(@theRes,u0(patches.i) ...
118 ,optimoptions('fsolve','Display','off'));
119 solveTime = toc
120 normResidual = norm(theRes(uSoln))
121 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.

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

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

```
141 figure(1), clf, colormap(0.8* hsv)
142 x(end+1,:,:)=nan; u0(end+1,:,:)=nan;
143 y(:,end+1,:)=nan; u0(:,end+1,:)=nan;
144 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.

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

4.8.1 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 .

```

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

```

Set Dirichlet boundary value of zero around the square domain.

```

184 u( 1 ,:,:, :, 1 ,:) = 0; % left edge of left patches
185 u(end,:,:,:,end,:) = 0; % right edge of right patches
186 u(:, 1 ,:,:, :, 1 ) = 0; % bottom edge of bottom patches
187 u(:,end,:,:, :,end) = 0; % top edge of top patches

```

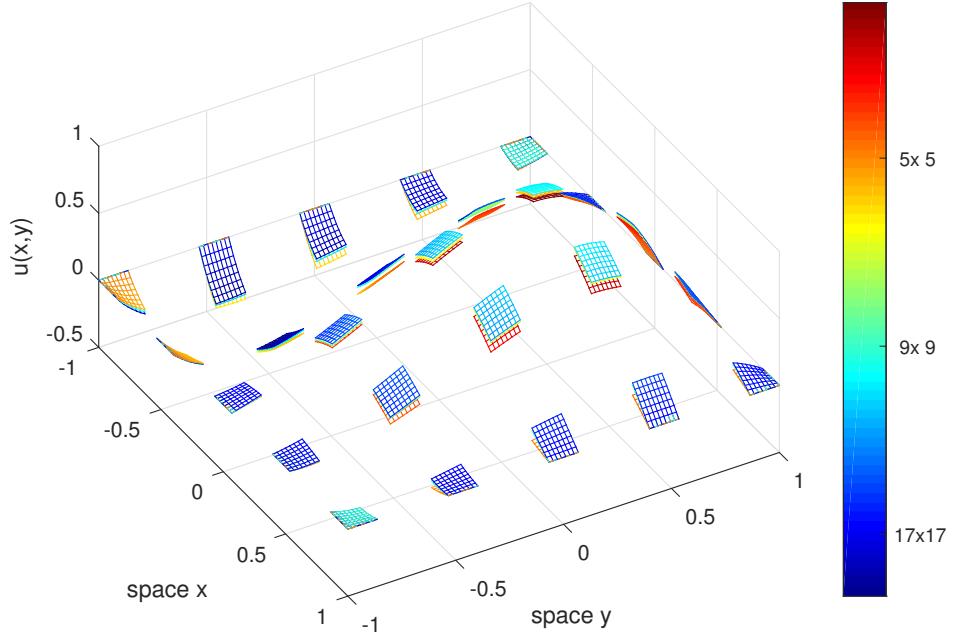
Compute the time derivatives via stored forcing and coefficients. Easier to code by conflating the last four dimensions into the one $,:$.

```

195 ut(i,j,:) ...
196 = 2*diff(u(:,j,:),2,1)/dx^2 +2*diff(u(:,j,:),2,2)/dy^2 ...
197 +2*patches.cs(i,j).*( u(i+1,j+1,:)-u(i-1,j+1,:)) ...
198 -(u(i+1,j-1,:)+u(i-1,j-1,:))/(4*dx*dy) ...
199 -patches.fu(i,j,:);
200 end%function twoscaleDiffForce2

```

Figure 4.7: 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 4.9). We only compare solutions only in these 25 common patches.



4.9 twoscaleDiffEquil2Errs: errors in equilibria of a 2D two-scale heterogeneous diffusion via small patches

Here we find the steady state $u(x, y)$ to the heterogeneous PDE (inspired by Freese et al.¹¹ §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 some microscale period ϵ (here $\epsilon \approx 0.24, 0.12, 0.06, 0.03$), of

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

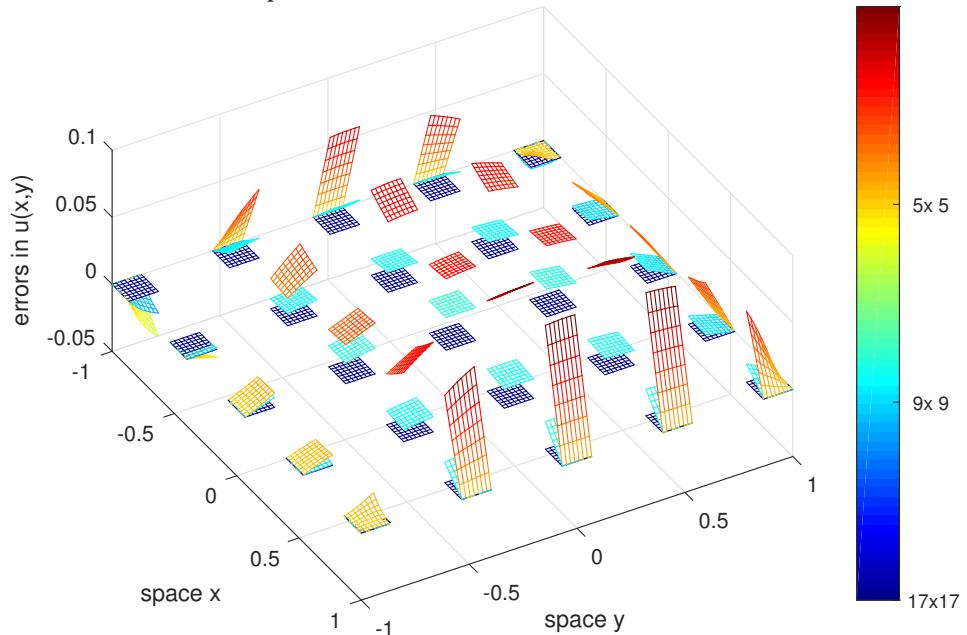
and for forcing $f := 10(x + y + \cos \pi x)$ (for which the solution has magnitude up to one).¹²

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

¹¹ <http://arxiv.org/abs/2211.13731>

¹² 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.¹³ For the same reason we do not invoke their smaller $\epsilon \approx 0.01$.

Figure 4.8: 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 4.9). 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).

```

81 clear all
82 global patches
83 %global OurCf2eps, OurCf2eps=true %option to save plot
84 switch 1
85     case 1, Dom.type = 'equispace'
86     case 2, Dom.type = 'chebyshev'
87     case 3, Dom.type = 'usergiven'
88 end% switch
89 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.

```

100 mPeriod = 6
101 z = (0.5:mPeriod)'/mPeriod;
102 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:

```

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

```

Set the periodicity ϵ , and other microscale parameters.

```

120 nPeriodsPatch = 1 % any integer
121 nSubP = nPeriodsPatch*mPeriod+2 % for edgy int
122 epsilon = 2/(nPatchMax*nPeriodsPatch+1/mPeriod)
123 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.

```

136 us=[]; xs=[]; ys=[]; nPs=[];
137 for log2N=log2Nmax:-1:2
138     if log2N==log2Nmax
139         Ps=linspace(1,nPatchMax ...
140             ,5-2*all(Dom.type=='chebyshev'))
141     else Ps=(Ps+1)/2
142 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 4.9.1](#).

```

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 3.19](#)).

```

207     tic;
208     maxIt = ceil(nVariables/10);
209     rhsb = theRes( zeros(size(patches.i)) );
210     [uSoln,flag] = bicgstab(@(u) rhsb-theRes(u),rhsb ...
211                             ,1e-9,maxIt,[],[],u0(patches.i));
212     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.

```

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

```

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

```

237     tic
238     [L,U] = ilu(Jac,struct('type','ilutp','droptol',1e-4));
239     LUfillFactor = (nnz(L)+nnz(U))/nnz(Jac)

```

```

240      [uSoln,flag] = bicgstab(@(u) rhsb-theRes(u),rhsb ...
241                      ,1e-9,maxIt,L,U,u0(patches.i));
242      precondSolveTime=toc
243      assert(flag==0,'preconditioner fails bicgstab. Lower droptol?')
244 end%if flag

```

Store the solution into the patches, and give magnitudes—Inf norm is $\max(\text{abs}())$.

```

251      normResidual = norm(theRes(uSoln),Inf)
252      normSoln = norm(uSoln,Inf)
253      u0(patches.i) = uSoln;
254      u0 = patchEdgeInt2(u0);
255      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 = [nP;nP];

```

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)
311 colorbar('Ticks',1:size(u,3) ...
312     , 'TickLabels', [num2str(nPs) ['x';'x';'x'] num2str(nPs)]);
313 xlabel('space $x$'), ylabel('space $y$'), zlabel('$u(x,y)$')
314 if0urCf2eps([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.

```

326 err=u(:,:,:,1)-u;
327 maxAbsErr=max(abs(err(:)));
328 figure(2), clf, colormap(jet)
329 for p=1:size(u,3)
330     mesh(x(:),y(:),err(:,:,p)',p+err(:,:,p)'/maxAbsErr);
331     hold on;
332 end, hold off
333 view(60,55)
334 colorbar('Ticks',1:size(u,3) ...
335     , 'TickLabels', [num2str(nPs) ['x';'x';'x'] num2str(nPs)]);
336 xlabel('space $x$'), ylabel('space $y$')
337 zlabel('errors in $u(x,y)$')
338 if0urCf2eps(mfilename)%optionally save

```

4.9.1 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 .

```

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

```

Set Dirichlet boundary value of zero around the square domain.

```

369 u( 1 ,:,:,:,:, 1 ,:) = 0; % left edge of left patches
370 u(end,:,:,:,end,:) = 0; % right edge of right patches
371 u(:, 1 ,:,:,:,:, 1 ) = 0; % bottom edge of bottom patches
372 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 $,:$

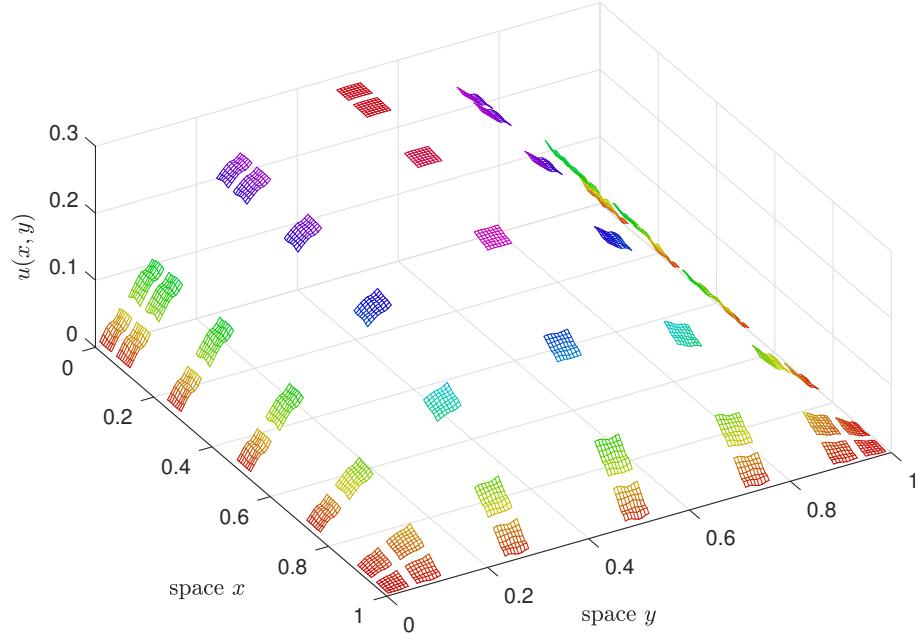
```

380 ut(i,j,:) ...
381 = 2*diff(u(:,j,:),2,1)/dx^2 +2*diff(u(i,:,:),2,2)/dy^2 ...
382     +2*patches.cs(i,j).*( u(i+1,j+1,:) -u(i-1,j+1,:) ...

```

```
383      -u(i+1,j-1,:) +u(i-1,j-1,:) )/(4*dx*dy) ...
384      +patches.fu(i,j,:);
385  end%function twoscaleDiffForce2
```

Figure 4.9: Equilibrium of the macroscale diffusion problem of Abdulle with boundary conditions of Dirichlet zero-value except for $x = 0$ which is Neumann (Section 4.10). Here the patches have a Chebyshev-like spatial distribution. The patch size is chosen large enough to see within.



4.10 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 et al. 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 4.9](#) shows solutions have some nice microscale wiggles reflecting the heterogeneity.

Clear, and initiate globals.

```
38 clear all
39 global patches
40 %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.)

```

53 mPeriod = 6
54 x = (0.5:mPeriod)'/mPeriod; y=x';
55 a = (2+1.8*sin(2*pi*x))./(2+1.8*sin(2*pi*y)) ...
56 +(2+ sin(2*pi*y))./(2+1.8*sin(2*pi*x));
57 diffusivityRange = [min(a(:)) max(a(:))]

```

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

```

64 epsilon = 0.04
65 dx = epsilon/mPeriod
66 nPeriodsPatch = 1 % any integer
67 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 4.10.1](#)

```

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 3.19](#)), 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.

```

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

```

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

```

150 mesh(patches.x(:),patches.y(:,u')); view(60,55)
151 xlabel('space $x$'), ylabel('space $y$'), zlabel('$u(x,y)$')
152 if0urCf2eps(mfilename) %optionally save plot

```

4.10.1 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 .

```

171 function ut = abdulleDiffForce2(t,u,patches)
172     dx = diff(patches.x(2:3)); % x space step
173     dy = diff(patches.y(2:3)); % y space step
174     i = 2:size(u,1)-1; % x interior points in a patch
175     j = 2:size(u,2)-1; % y interior points in a patch
176     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.

```

184     u( 1 ,:,:, :, 1 ,:) = 0; % left edge of left patches
185     u(end,:,:,:,end,:) = 0; % right edge of right patches
186     u(:, 1 ,:,:, :, 1 ) = 0; % bottom edge of bottom patches
187     u(:,end,:,:,:,end) = 0; % top edge of top patches
188     if 1, u(1,:,:,:,1,:) = u(2,:,:,:,1,:); end% left Neumann

```

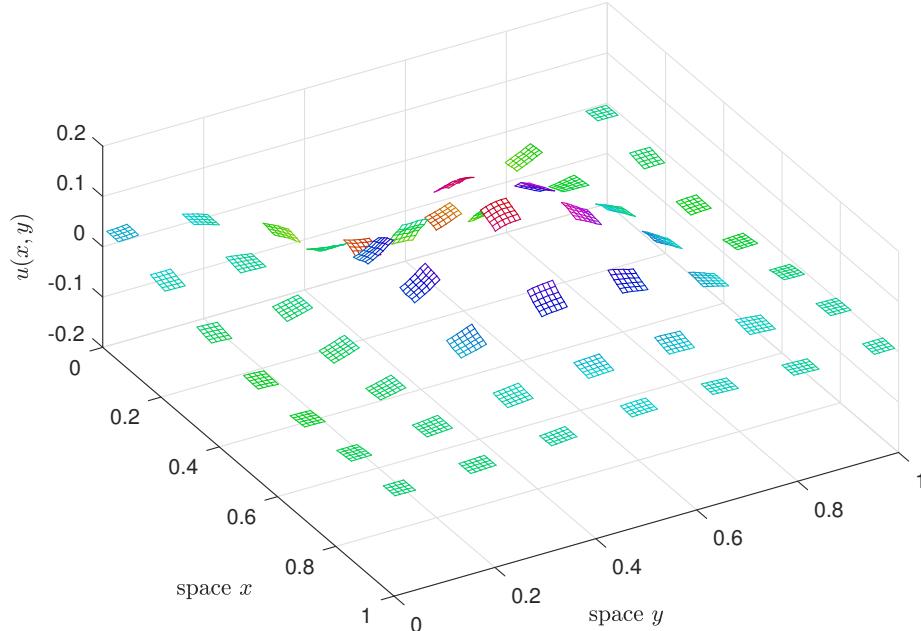
Compute the time derivatives via stored forcing and coefficients. Easier to code by conflating the last four dimensions into the one $,:$.

```

196     ut(i,j,:) = diff(patches.cs(:,j).*diff(u(:,j,:)))/dx^2 ...
197         + diff(patches.cs(i,:).*diff(u(i,:,:),1,2),1,2)/dy^2 ...
198         + 10;
199 end%function abdulleDiffForce2

```

Figure 4.10: Equilibrium of the macroscale diffusion problem of Bonizzoni et al. with Neumann boundary conditions of zero (Section 4.11). Here the patches have a equispaced spatial distribution. The microscale periodicity, and hence the patch size, is chosen large enough to see within.



4.11 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.¹⁴ §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, $\mu_1(x, y) \in [0.01, 0.1]$ ¹⁵ 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 4.10 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.

```
50 clear all
51 global patches
52 %global OurCf2eps, OurCf2eps=true %option to save plot
```

¹⁴ <http://arxiv.org/abs/2211.15221>

¹⁵ More interesting microscale structure arises here for μ_1 a factor of three smaller.

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

```

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

```

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

```

74 epsilon = 0.04
75 dx = epsilon/mPeriod
76 nPeriodsPatch = 1 % any integer
77 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:

```

89 nPatch = 7
90 Dom.type= 'equispace';
91 Dom.bcOffset = 0.5;
92 configPatches2(@randAdvecDiffForce2,[0 1],Dom ...
93 ,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 4.11.1](#).

```

101 mu = [ 0.25+0.5*rand(1,2) 0.1+0.15*rand ]
102 patches.fu = exp(-((patches.x-mu(1)).^2 ...
103 +(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.

```

118 u0 = zeros(nSubP,nSubP,1,1,nPatch,nPatch);
119 u0([1 end],:,:) = nan; u0(:,[1 end],:) = nan;
120 patches.i = find(~isnan(u0));
121 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 3.19](#)).

```

130 tic;
131 uSoln = fsolve(@theRes,u0(patches.i) ...
132 ,optimoptions('fsolve','Display','off'));
133 solnTime = toc

```

```

134 normResidual = norm(theRes(uSoln))
135 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.

```

143 u0(patches.i) = uSoln;
144 u0 = patchEdgeInt2(u0);

```

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

```

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

```

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

```

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

```

4.11.1 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 .

```

187 function ut = randAdvecDiffForce2(t,u,patches)
188     dx = diff(patches.x(2:3)); % x space step
189     dy = diff(patches.y(2:3)); % y space step
190     i = 2:size(u,1)-1; % x interior points in a patch
191     j = 2:size(u,2)-1; % y interior points in a patch
192     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.

```

200     u( 1 ,:,:, :, 1 ,:) = u( 2 ,:,:, :, 1 ,:); % left edge of left patches
201     u(end,:,:,:,end,:) = u(end-1,:,:,:,end,:); % right edge of right patches
202     u(:, 1 ,:,:, :, 1 ) = u(:, 2 ,:,:, :, 1 ); % bottom edge of bottom patches
203     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 $,:$.

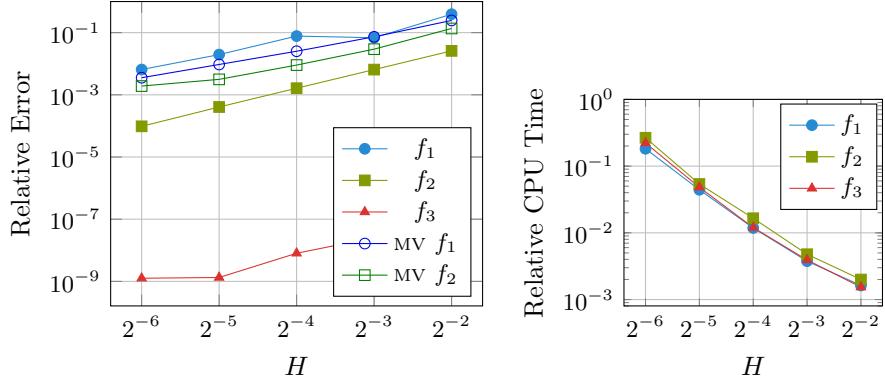
```

211     ut(i,j,:)
212     = patches.cs(i,j,1).*(diff(u(:,j,:),2,1)/dx^2 ...
213         +diff(u(:, :,1),2,2)/dy^2) ...
214         -patches.cs(i,j,2).*(u(i+1,j,:)-u(i-1,j,:))/(2*dx) ...

```

```
215      -patches.cs(i,j,3).*(u(i,j+1,:)-u(i,j-1,:))/(2*dy) ...
216      -u(i,j,:)+patches.fu(i,j,:);
217  end%function randAdvecDiffForce2
```

Figure 4.11: results for the computational homogenisation of a forced, non-autonomous, 2D wave (Section 4.12). (left) relative RMS error of the patch scheme, each patch of width $1/128$, as a function of patch spacing H . The unfilled symbols are those of the energy norm from Maier & Verfürth (2021) (their Figure 5.1). (right) the relative compute time decreases very quickly in H as there are fewer patches spaced further apart.



4.12 homoWaveEdgy2: computational homogenisation of a forced, non-autonomous, 2D wave via simulation on small patches

This section extends to 2D waves, in a microscale heterogeneous media, the 2D diffusion code discussed in Section 4.5. It favourably compares to the examples of Maier & Verfürth (2021).

Figure 4.11 summarises the results here. The left (larger) graph shows the error in the patch scheme decreasing with decreasing patch spacing H (increasing number of patches). Forcing f_1 and f_2 are as specified by §5.1 of Maier & Verfürth (2021), whereas f_3 here is f in their §5.2. For the case of forcing f_1 which is discontinuous in space (at $x = 0.4$), the errors are similar to that of Maier & Verfürth (2021)—compare the filled with unfilled circles. For the case of forcing f_2 which is continuous in the spatial domain, except for a second derivative discontinuity in its odd-periodic extension, the errors of the patch scheme are an order of magnitude better than that of Maier & Verfürth (2021)—compare the filled with unfilled squares. For the case of forcing f_3 which is smooth in the domain and in its odd-periodic extension, the patch scheme errors, roughly 10^{-8} , are at the tolerance of the time integration. Two caveats in a comparison with Maier & Verfürth (2021) are the slightly different norms used, and that they also address errors in the time integration, whereas here we use a standard adaptive integrator in order to focus purely on the spatial errors of the patch scheme.

Now let's code the simulation of the forced, non-autonomous, 2D wave. Maier & Verfürth (2021) have Dirichlet BCs of zero around the unit square, so replicate here by the odd periodic extension to the spatial domain $[-1, 1]^2$. In their §5.1, their microscale mesh step is $1/512 = 2^{-9}$. Coding that here results in a compute time of roughly 90 minutes, so here I provide a much coarser case that computes in only a few minutes: change as you please.

```

68 clear all
69 dx = 1/128 % 1/512=2^{-9} is the original, but takes 90 mins

```

The heterogeneity is of period four on the microscale lattice, so code a minimal patch size that covers one period.

```

77 epsilon = 4*dx
78 nPeriodsPatch = 1
79 mPeriod = round(epsilon/dx)
80 nSubP = mPeriod*nPeriodsPatch+2

```

Choose which of three forcing functions to use

```
86 fn=2
```

[Maier & Verfürth \(2021\)](#) use varying number of macroscale grid steps from 4 to 64 on $[0, 1]$ so here on $[-1, 1]$ we use double the number patches in each direction. Loop over the number of patches used, starting with the full domain simulation, and then progressively coarsening the macroscale grid of patches.

```

99 nPatch = 2/epsilon/nPeriodsPatch
100 for iPAt=0:9
101 if iPAt>0, nPatch=nPatch/2, end
102 if nPatch<8, break, end

```

Set the periodic heterogeneous coefficient, isotropic:

$$a_\epsilon(t, x) = [3 + \sin(2\pi x/\epsilon) + \sin(2\pi t)] \cdot [3 + \sin(2\pi y/\epsilon) + \sin(2\pi t)],$$

which being in product form with two time-dependencies we store as the two spatially varying factors—although to preserve odd symmetry we phase shift the heterogeneity from sines to cosines. It is a user’s choice whether to code such spatial dependencies here with `cHetr` or within the time derivative function itself. In this case, I choose to code microscale heterogeneous coefficients here via `cHetr`, and the macroscale variation of f_i in the time derivative function.

Here the period of the heterogeneity is only four microscale lattice points in each direction (which is pretty inaccurate on the microscale, but immaterial as we and [Maier & Verfürth \(2021\)](#) only compare to the coded system on the microscale lattice, not to the PDE). With the following careful choices we ensure all the hierarchy of patch schemes both maintain odd symmetry, and also compute on grid points that are common with the full domain.

```

130 ratio = (nSubP-2)*dx/(2/nPatch)
131 Xleft=(1-ratio)/nPatch;
132 xmid=Xleft+dx*(0:mPeriod-1)'; % half-points
133 xi = Xleft+dx*(-0.5:mPeriod-1)'; % grid-points
134 % two components for ax, the x-dirn interactions
135 cHetr(:,:,1) = (3+cos(2*pi*xmid/epsilon))+0*xi';
136 cHetr(:,:,2) = 0*xmid+(3+cos(2*pi*xi'/epsilon));
137 % two components for ay, the y-dirn interactions
138 cHetr(:,:,3) = (3+cos(2*pi*xi/epsilon))+0*xmid';
139 cHetr(:,:,4) = 0*xi+(3+cos(2*pi*xmid'/epsilon));

```

Configure patches using spectral interpolation. Quadratic interpolation did not seem significantly different for the case of discontinuous forcing f_1 .

```
148 configPatches2(@heteroWave2, [-1 1 -1 1], nan, nPatch ...
149     , 0, ratio, nSubP, 'EdgyInt', true, 'hetCoeffs', cHetr );
```

A check on the spatial geometry.

```
155 global patches
156 dxPat=diff(patches.x(1:2));
157 assert(abs(dx-dxPat)<1e-9, "dx mismatch")
```

Simulate Set the particular forcing function to use, and the zero initial conditions of a simulation.

```
167 patches.eff=fn;
168 clear uv0
169 uv0(:,:,1,1,:,:)= 0*patches.x+0*patches.y;
170 uv0(:,:,2,1,:,:)= 0*patches.x+0*patches.y;
```

Integrate using standard integrators. [Maier & Verfürth \(2021\)](#) use a scheme with fixed time-step of $\tau = 2^{-7} = 1/128$. Here `ode23` uses variable steps of about 0.0003, and takes 7 s for `nPatch=2*4` (whereas `ode15s` takes 149 s—even for the dissipating case), and takes 287 s for `nPatch=2*32` and roughly 4000 s for full domain `nPatch=2*128`.

```
182 disp('Now simulate over time')
183 tic
184 [ts,us] = ode23(@patchSys2, linspace(0,1,11), uv0(:));
185 if iPAt==0, odeTime0=toc
186 else relodeTime(iPat)=toc/odeTime0
187 end
```

Compute error compared to full domain simulation Get spatial coordinates of patch-interior points, and reshape to column vectors.

```
197 i = 2:nSubP-1;
198 x = squeeze(patches.x(i,:,:,:,:,:));
199 y = squeeze(patches.y(:,i,:,:,:,:));
200 x=x(:); y=y(:);
```

At the final time of $t = 1$, get the row vector of data, form into the 6D array via the interpolation to the edges, and reshape patch-interior points to 2D spatial array.

```
208 uv = squeeze(patchEdgeInt2(us(end,:)));
209 u = squeeze(uv(i,i,1,:,:));
210 u = reshape(permute(u,[1 3 2 4]),[numel(x) numel(y)]);
```

If this is the full domain simulation, then store as the reference solution.

```
217 if iPAt==0
218 x0=x; y0=y; u0=u;
```

```

219     rms0=sqrt(mean(u0(:).^2))
220 else
    Else compute the error compared to the full domain solution. First find
    the indices of the full domain that match the spatial locations of the patch
    scheme.
228     [i,k] = find(abs(x0-x')<1e-9);
229     assert(length(i)==length(x),'find error in index i')
230     [j,k] = find(abs(y0-y')<1e-9);
231     assert(length(j)==length(y),'find error in index j')

```

The RMS error over the surface is

```

237     errs=u-u0(i,j);
238     relrmserr(iPat)=sqrt(mean(errs(:).^2))/rms0
239     H(iPat)=2/nPatch
240 end%if iPat

```

End the loop over the various number of patches, and return. Further, here not executed, code in the file animates the solution over time, and computes spectrum of the system.

```

250 end%for iPat
251 figure(1), clf
252 loglog(H,relrmserr,'o:'), grid on
253 xlabel('$H$'), ylabel('relative error')
254 return

```

4.12.1 heteroWave2(): heterogeneous Waves

This function codes the lattice heterogeneous waves inside the patches. The forced wave PDE is

$$u_t = v, \quad v_t = \vec{\nabla}(a\vec{\nabla} \cdot u) + f$$

for scalars $a(t, x, y)$ and $f(t, x, y)$ where a has microscale variations. For 6D input arrays u , x , and y (via edge-value interpolation of `patchSys2`, [Section 4.2](#)), computes the time derivative at each point in the interior of a patch, output in ut . The four 2D arrays of heterogeneous interaction coefficients, c_{ijk} , have previously been stored in `patches.cs` (3D).

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

```

26 function ut = heteroWave2(t,u,patches)
27 if nargin<3, global patches, end

```

Microscale space-steps, and interior point indices.

```

33 dx = diff(patches.x(2:3)); % x micro-scale step
34 dy = diff(patches.y(2:3)); % y micro-scale step
35 i = 2:size(u,1)-1; % x interior points in a patch
36 j = 2:size(u,2)-1; % y interior points in a patch
37 assert(max(abs(u(:)))<9999,"u-field exploding")

```

Form coefficients here—odd periodic extension. To avoid slight errors in periodicity (in full domain simulation), first adjust any coordinates crossing $x = \pm 1$ or $y = \pm 1$.

```
47 x=patches.x; y=patches.y;
48 l=find(abs(x)>1); x(l)=x(l)-sign(x(l))*2;
49 l=find(abs(y)>1); y(l)=y(l)-sign(y(l))*2;
```

Then set at this time three possible forcing functions, although only use one depending upon `patches.eff`. Forcing f_1 and f_2 are as specified by §5.1 of [Maier & Verfürth \(2021\)](#), whereas f_3 here is f in their §5.2.

```
59 f1 = ( (abs(x)>0.4)*(20*t+230*t^2) ...
60     +(abs(x)<0.4)*(100*t+2300*t^2) ).*sign(x).*sign(y);
61 f2 = 20*t*x.* (1-abs(x)).*y.* (1-abs(y)) ...
62     +230*t^2*(sign(y).*x.* (1-abs(x))+sign(x).*y.* (1-abs(y)));
63 f3 = (5*t+50*t^2)*sin(pi*x).*sin(pi*y);
```

Also set the heterogeneous interactions at this time.

```
69 ax = (patches.cs(:,:,1)+sin(2*pi*t)) ...
70     .* (patches.cs(:,:,2)+sin(2*pi*t));
71 ay = (patches.cs(:,:,3)+sin(2*pi*t)) ...
72     .* (patches.cs(:,:,4)+sin(2*pi*t));
```

Reserve storage (using `nan+u` appears quickest), and then assign time derivatives for interior patch values due to the heterogeneous interaction and forcing.

```
81 ut = nan+u; % preallocate output array
82 ut(i,j,1,:) = u(i,j,2,:);
83 ut(i,j,2,:) ...
84 = diff(ax(:,j).*diff(u(:,j,1,:),1),1)/dx^2 ...
85     +diff/ay(i,:).*diff(u(i,:,1,:),1,2),1,2)/dy^2 ...
86     +(patches.eff==1)*f1(i,j,:,:)
87     +(patches.eff==2)*f2(i,j,:,:)
88     +(patches.eff==3)*f3(i,j,:,:)
89     + 1e-4*(diff(u(:,j,2,:),2,1)/dx^2+diff(u(i,:,2,:),2,2)/dy^2);
90 end% function
```

In the last line above, the slight damping of 10^{-4} causes microscale modes to decay at rate e^{-28t} , with frequencies 2000–5000, whereas macroscale modes decay with rates roughly 0.0005–0.05 with frequencies 10–100. This slight damping term may correspond to the weak damping of the backward Euler scheme adopted by [Maier & Verfürth \(2021\)](#) for time integration.

4.13 SwiftHohenberg2dPattern: patterns of the Swift–Hohenberg PDE in 2D on patches

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Figures 4.12 to 4.17 show an example simulation in time generated by the patch scheme applied to the patterns arising from the 2D Swift–Hohenberg PDE.

Consider a lattice of values $u_i(t)$, with lattice spacing dx , and governed by a microscale centred discretisation of the Swift–Hohenberg PDE

$$\partial_t u = -(1 + \nabla^2/k_0^2)^2 u + \text{Ra} u - u^3, \quad (4.1)$$

with various boundary conditions at $x, y = 0, L$. For Ra just above critical, say $\text{Ra} = 0.1$, the system rapidly evolves to spatial quasi-periodic solutions with period ≈ 0.24 when wavenumber parameter $k_0 = 26$. These spatial oscillations are here resolved on a micro-grid of spacing 0.042. On medium times these spatial oscillations grow to near equilibrium amplitude of $\sqrt{\text{Ra}}$, and over very long times the phases of the oscillations evolve in space to adapt to the boundaries.

Set the desired microscale periodicity, and correspondingly choose random microscale diffusion coefficients (with subscripts shifted by a half).

```

42 clear all
43 cMap=jet(64); cMap=0.8*cMap(7:end-7,:); % set colormap
44 basename = ['r' num2str(floor(1e5*rem(now,1))) mfilename]
45 %global OurCf2eps, OurCf2eps=true %optional to save plots
46 Ra = 0.2 % Ra>0 leads to patterns
47 nGapFac = 2
48 waveLength = 0.5/nGapFac
49 nPtsPeriod = 6
50 dx = waveLength/nPtsPeriod
51 k0 = 2.1*pi/waveLength

```

The above factor 2.1 is close to $3/\sqrt{2} = 2.1213$ for which $(\pm 1, \pm 2)$ modes have same linear growth-rate as $(\pm 2, 0)$ modes.

Establish global data struct `patches` for the Swift–Hohenberg PDE on some square domain. For simplicity, use five patches in each direction. Quartic (fourth-order) interpolation `ordCC = 4` provides values for the inter-patch coupling conditions. Set `bcOffset` for different boundary conditions around the square domain.

```

67 nPatch = 5
68 nSubP = 2*nPtsPeriod+4
69 Len = nPatch;
70 ordCC = 4;
71 dom.type='equispace';
72 dom.bcOffset=[0.5 0.5;1.0 1.5]
73 patches = configPatches2(@SwiftHohenbergPDE, [0 Len], dom ...
74 ,nPatch,ordCC,dx,nSubP,'EdgyInt',true,'nEdge',2);
75 xs=squeeze(patches.x);
76 ys=squeeze(patches.y);
```

4.13.0.1 Simulate in time

Set an initial condition, and here integrate forward in time using a standard method for stiff systems. Integrate the interface `patchSys2` (Section 4.2) to the microscale differential equations (despite the extreme stiffness, `ode23` is ten times quicker than `ode15s`). Because pattern evolution is eventually phase-diffusion, here sample the pattern at quadratically varying times.

```

93 fprintf('\n**** Simulate in time\n')
94 u0 = 0.3*( -1+2*rand(size(patches.x+patches.y)) );
95 Ts=400*linspace(0,1,97).^2;
96 tic
97 [ts,us] = ode23(@patchSys2, Ts, u0(:),[], patches,k0,Ra);
98 simulateTime = toc
99 us = reshape(us',nSubP,nSubP,nPatch,nPatch,[]);
```

Plot the simulation such as that shown in Figures 4.12 to 4.17 First, reshape the data, omitting edge values.

```

135 xs([1:2 end-1:end],:) = nan;
136 ys([1:2 end-1:end],:) = nan;
137 us = reshape( permute(us,[1 3 2 4 5]) ...
138 ,nSubP*nPatch,nSubP*nPatch,[]);
139 uRange=[min(us(:)) max(us(:))];
```

Second, plot six examples of the evolving pattern, equi-spaced in time-index.

```

146 plots = round( 1+linspace(0,1,7)*(numel(ts)-1) )
147 for p=2:numel(plots)
148 figure(p),clf
149 mesh(xs(:,ys(:,us(:,:,plots(p)))')
150 axis equal, view(0,90)
151 caxis(uRange), colormap(cMap), colorbar
152 xlabel('space $x$'), ylabel('space $y$'), zlabel('$u(x,y,t)$')
153 title(['time = ' num2str(ts(plots(p)),3)])
```

Figure 4.12:
 pattern field $u(x, y, t)$ in the patch scheme applied to a microscale discretisation of the 2D Swift–Hohenberg PDE. At this early time much of the random sub-patch microstructure has decayed leaving some random marginal modes starting to grow.

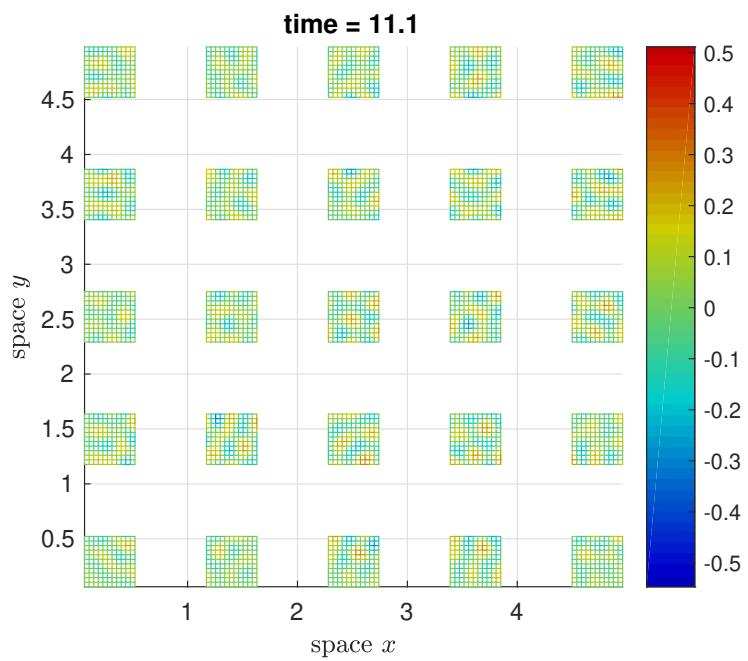


Figure 4.13:
 pattern field $u(x, y, t)$ in the patch scheme applied to a microscale discretisation of the 2D Swift–Hohenberg PDE. By now the local sub-patch patterns have reached a quasi-equilibrium amplitude.

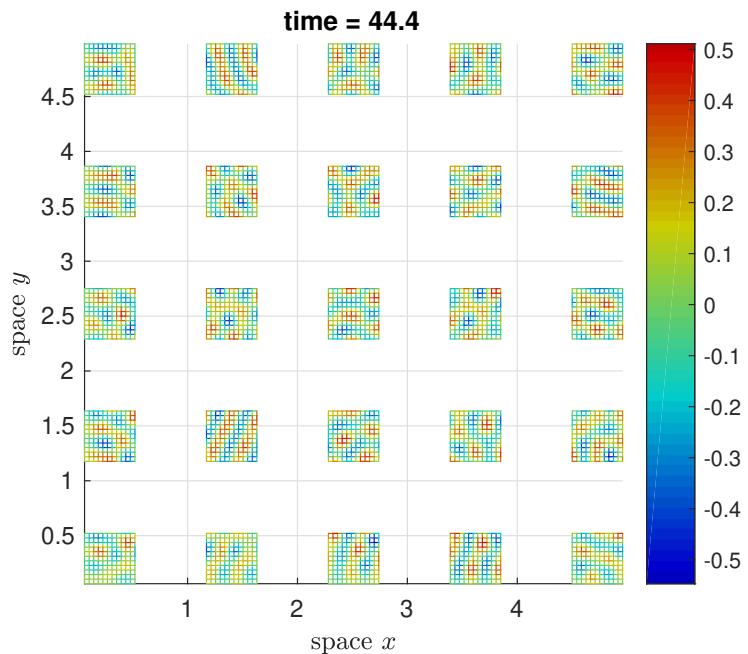


Figure 4.14:
 pattern field $u(x, y, t)$ in the patch scheme applied to a microscale discretisation of the 2D Swift–Hohenberg PDE. Patterns within the patches are evolving to the preferred rolls, but with weak coupling to other patches.

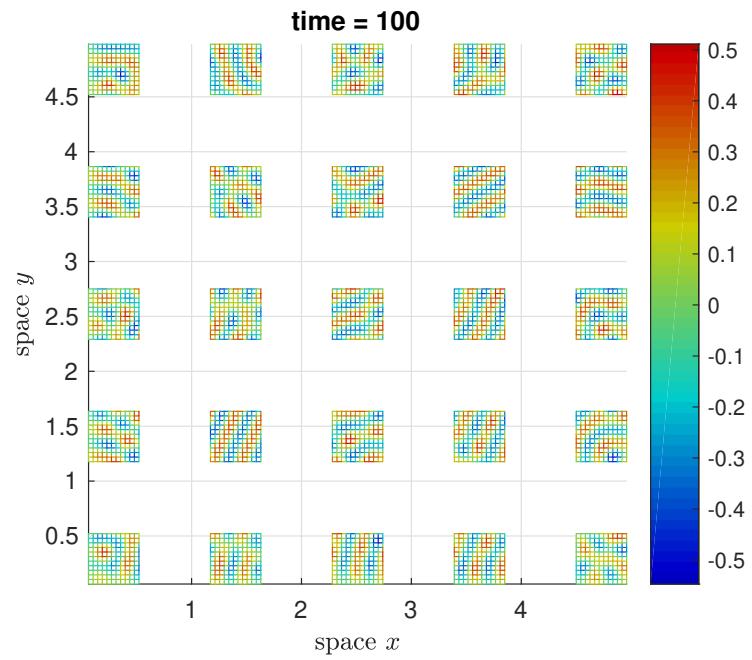


Figure 4.15:
 pattern field $u(x, y, t)$ in the patch scheme applied to a microscale discretisation of the 2D Swift–Hohenberg PDE. Can see different effects arising at different types of boundaries.

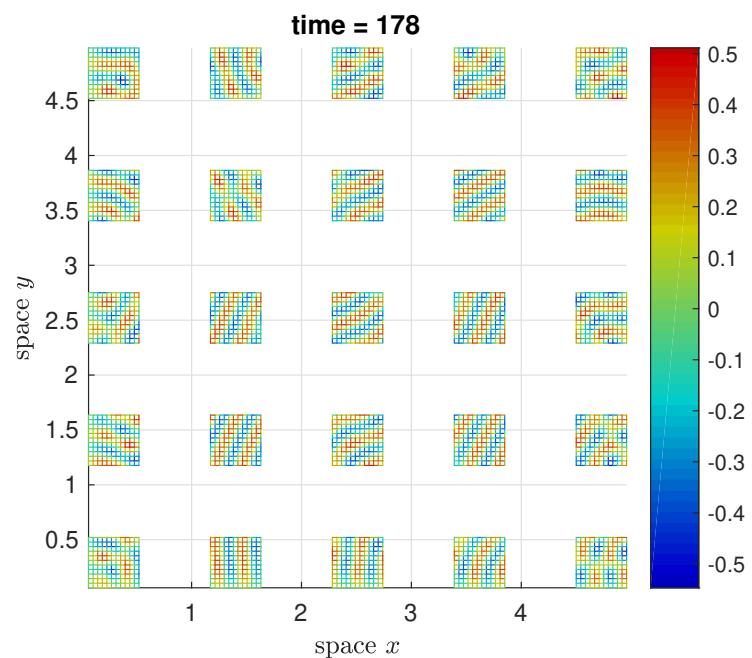


Figure 4.16:
 pattern field
 $u(x, y, t)$ in the
 patch scheme
 applied to a
 microscale dis-
 cretisation of
 the 2D Swift–
 Hohenberg PDE.

...

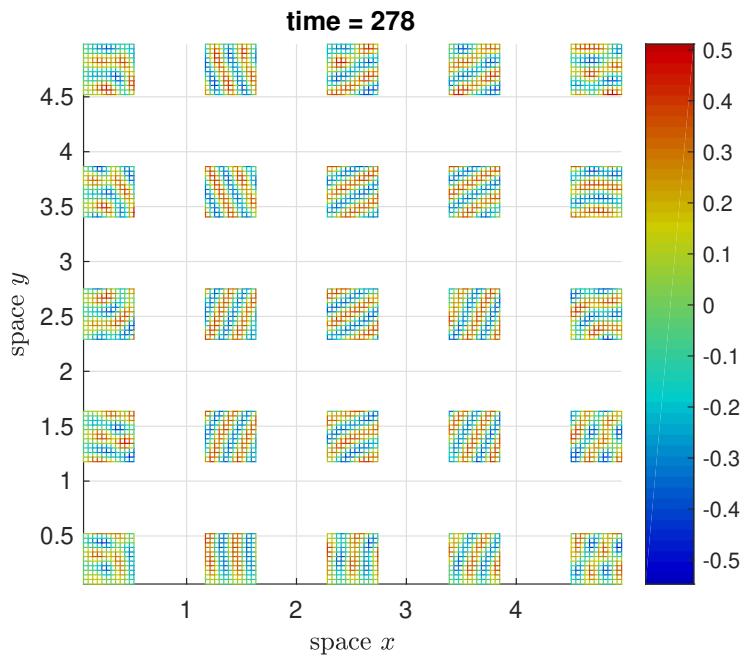
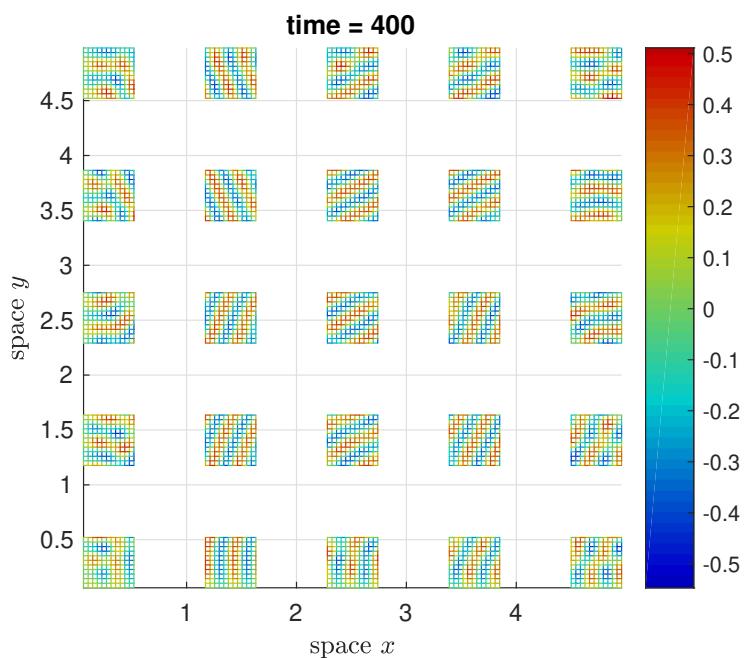


Figure 4.17:
 pattern field
 $u(x, y, t)$ in the
 patch scheme
 applied to a
 microscale dis-
 cretisation of
 the 2D Swift–
 Hohenberg PDE.

...



```

154     if0urCf2eps([basename num2str(p)], [12 11])
155 end%for p

```

Third, plot animation in time: starts after a key press.

```

161 %%
162 figure(1),clf
163 cf=mesh(xs(:,ys(:,us(:,:,1));
164 axis equal, view(0,90)
165 caxis(uRange), colormap(cMap), colorbar
166 xlabel('space $x$'), ylabel('space $y$'), zlabel('$u(x,y,t)$')
167 title(['time = ' num2str(ts(1),3)])
168 ca=gca;
169 disp('Press any key to start animation'), pause
170 for p=2:numel(ts)
171     cf.ZData=us(:,:,p)';
172     cf.CData=us(:,:,p)';
173     ca.Title.String=['time = ' num2str(ts(p),3)];
174     pause(0.1)
175 end

```

Fin.

4.13.1 The Swift–Hohenberg PDE and BCs inside patches

As a microscale discretisation of Swift–Hohenberg PDE $ut = -(1 + \nabla^2/k_0^2)^2 u + Ra u - u^3$, here code straightforward centred discretisation in space.

```

189 function ut=SwiftHohenbergPDE(t,u,patches,k0,Ra)
190     dx=diff(patches.x(1:2)); % microscale spacing
191     dy=diff(patches.y(1:2)); % microscale spacing
192     i=3:size(u,1)-2; % interior points in patches
193     j=3:size(u,2)-2; % interior points in patches

```

Code various boundary conditions. For slightly simpler coding, squeeze out the two singleton dimensions.

```

200     u = squeeze(u);
201     u(1:2,:,1,:)=0; % u=u_x=0 at x=0
202     u(:,1:2,:,1)=0; % u=u_y=0 at y=0
203     u(end-1,:,:,:)=0; % u=0 at x=L
204     u(end ,:,:,:)=-u(end-2,:,:,:); % u_x=0 at x=L
205     u(:,end-1,:,:,:)=u(:,end-2,:,:,:); % u_y=0 at y=L
206     u(:,end ,:,:,:)=u(:,end-3,:,:,:); % u_yyy=0 at y=L

```

Here code straightforward centred discretisation in space.

```

212     ut=nan+u; % preallocate output array
213     v = u(2:end-1,2:end-1,:,:,:) ...
214         +( diff(u(:,2:end-1,:,:,:),2,1)/dx^2 ...
215             +diff(u(2:end-1,:,:,:),2,2)/dy^2 )/k0^2;
216     ut(i,j,:,:,:) = -( v(2:end-1,2:end-1,:,:,:) ...
217         +( diff(v(:,2:end-1,:,:,:),2,1)/dx^2 ...

```

```

218      +diff(v(2:end-1,:,:,:),2,2)/dy^2 )/k0^2 ) ...
219      +Ra*u(i,j,:,:)-u(i,j,:,:).^3;
220  end

```

4.13.2 patchEdgeInt2test: tests 2D patch coupling

A script to test the spectral, finite-order, and divided difference, polynomial interpolation of function `patchEdgeInt2()`. Tests one or several variables, normal grids, and also tests centre and edge interpolation. But does not yet test staggered grids, core averaging, etc as they are not yet implemented.

Start by establishing global data struct for the range of various cases. Choose a number of realisations for every type.

```

21 clear all, close all
22 global patches
23 nRealise = 20

```

4.13.2.1 Check divided difference interpolation

```

36 fprintf('\n\n**** Check divided difference interpolation\n')
37 pause(1)

```

Check over various types and orders of interpolation, numbers of patches, random domain lengths, random ratios, and randomised distribution of patches. (The `@sin` is a dummy.)

```

46 maxErrors=[];
47 for realisation = 1:nRealise
48     nEdge = randi(3,1,2)% =1,2, or 3
49     edgyInt = (rand>0.5)
50     Lx = 1+3*rand; Ly = 1+3*rand;
51     xyLim = [0 Lx 0 Ly]-[rand*[1 1] rand*[1 1]]
52     nSubP = nEdge.*((2-edgyInt)*randi(3,1,2)+1+edgyInt )
53     ordCC = 2*randi(4)
54     nPatch = ordCC+randi(4,1,2)
55     dx = [Lx Ly]./nPatch./nSubP.*rand(1,2)/2
56     configPatches2(@sin,xyLim,'equispace',nPatch,ordCC ...
57 ,dx,nSubP,'EdgyInt',edgyInt,'nEdge',nEdge);

```

Second, displace patches to a random non-uniform spacing.

```

63 Hx = diff(patches.x(1,1,:,:,:1:2,1));
64 patches.x = patches.x+0.8*Hx*(rand(1,1,1,1,nPatch(1),1)-0.5);
65 Hx = squeeze( diff(patches.x(1,1,:,:,:1)) );% for information only
66 Hy = diff(patches.y(1,1,:,:,:1:2));
67 patches.y = patches.y+0.8*Hy*(rand(1,1,1,1,1,nPatch(2))-0.5);
68 Hy = squeeze( diff(patches.y(1,1,:,:,:1,:)) );% for information only

```

Check multiple fields simultaneously Set profiles to be various powers of x and y , ps and qs , and store as different ‘variables’ at each point. First,

limit the order of test polynomials by the order of interpolation and by the number of patches.

```

81      ox=min(ordCC,nPatch(1)-1);
82      oy=min(ordCC,nPatch(2)-1);
83      [ps,qs]=ndgrid(0:ox,0:oy);
84      ps=reshape(ps,1,1,[]);
85      qs=reshape(qs,1,1,[]);
86      cs=2*rand(size(ps))-1;
87      u0=cs.*patches.x.^ps.*patches.y.^qs;

```

Then evaluate the interpolation, setting edges to `inf` for error checking.

```

94      u=u0;
95      u([1:nEdge(1) end-nEdge(1)+1:end],:,:)=inf;
96      u(:,[1:nEdge(2) end-nEdge(2)+1:end],:,:)=inf;
97      ui=patchEdgeInt2(u(:));

```

All patches should have zero error: but need to either in `patchEdgeInt2` comment out NaN assignment of boundary values, or not test the two extreme patches here, or add code to omit NaNs here. High-order interpolation seems to be more affected by round-off so relax error size.

```

107      error = ui-u0;
108      hist(log10(abs(error(abs(error)>1e-20))),-20:-7)
109      xlabel('log10 error'), pause(0.3)%??
110      maxError=max(abs(error(:)))
111      maxErrors=[maxErrors maxError];
112      assert(maxError<3e-12*4^ordCC ...
113      , 'failed divided difference interpolation')
114      disp('*** This divided difference test passed')

```

End the for-loops over various parameters.

```

121  end% for realisation
122  maxMaxErrorDividedDiffs = max(maxErrors)
123  disp('***** Passed all divided difference interpolation')
124  pause(1)

```

4.13.2.2 Test standard spectral interpolation

```

138  fprintf('\n\n**** Test standard spectral interpolation\n')
139  pause(1)

```

Test over various numbers of patches, random domain lengths and random ratios. Try realisations of random tests.

```

146  for realisation=1:nRealise

```

Choose and configure random sized domains, random sub-patch resolution, random size-ratios, random number of periodic-patches, randomly edge or mid-patch interpolation.

```

154 nEdge=randi(3,1,2)% =1,2, or 3
155 edgyInt = (rand>0.5)
156 Lx = 1+3*rand, Ly = 1+3*rand
157 xyLim = [0 Lx 0 Ly]-[rand*[1 1] rand*[1 1]]
158 nSubP = nEdge.*((2-edgyInt)*randi(3,1,2)+1+edgyInt )
159 nPatch = randi([3 6],1,2)
160 dx = [Lx Ly]./nPatch./nSubP.*rand(1,2)/2
161 configPatches2(@sin,xyLim,'periodic',nPatch,0 ...
162 ,dx,nSubP,'EdgyInt',edgyInt,'nEdge',nEdge);

```

Choose a random number of fields, then generate trigonometric shape with random wavenumber and random phase shift. But if an even number of patches in either direction, then do not test the highest wavenumber because of aliasing problem.

```

172 nV=randi(3)
173 [nx,Nx]=size(squeeze(patches.x));
174 [ny,Ny]=size(squeeze(patches.y));
175 u0=nan(nx,ny,nV,1,Nx,Ny);
176 for iV=1:nV
177     kx=randi([0 floor((nPatch(1)-1)/2)])
178     ky=randi([0 floor((nPatch(2)-1)/2)])
179     phix=pi*rand*(2*kx~=nPatch(1))
180     phiy=pi*rand*(2*ky~=nPatch(2))
181     % generate 6D array via auto-replication
182     u0(:,:,:iV,1,:,:)=sin(2*pi*kx*patches.x/Lx+phix) ...
183             .*sin(2*pi*ky*patches.y/Ly+phiy);
184 end

```

Copy and `nan` the edges, then interpolate

```

190 u=u0;
191 u([1:nEdge(1) end-nEdge(1)+1:end],:,:)=nan;
192 u(:,[1:nEdge(2) end-nEdge(2)+1:end],:,:)=nan;
193 u=patchEdgeInt2(u(:));

```

Compute difference. If there is an error in the interpolation, then abort the script for checking: please record parameter values and inform us.

```

201 error = u-u0;
202 assert(all(~isnan(error(:))), 'found nans in the error!')
203 hist(log10(abs(error(abs(error)>1e-20))), -20:-7)
204 xlabel('log10 error'), pause(0.3)%??
205 normError=norm(error(:))
206 assert(normError<1e-12, '2D spectral interpolation failed')
207 disp('*** This spectral test passed')

```

End the for-loop over realisations

```

214 end
215 disp('***** All the spectral tests passed')
216 pause(1)

```

4.13.2.3 Check polynomial finite width interpolation

Check over various types and orders of interpolation, numbers of patches, random domain lengths and random ratios. (The `@sin` is a dummy.)

```

234 for realisations=1:nRealise
235     nEdge = randi(3,1,2)% =1,2, or 3
236     edgyInt = (rand>0.5)
237     nSubP = nEdge.*((2-edgyInt)*randi(3,1,2)+1+edgyInt )
238     ordCC = 2*randi(4)
239     nPatch = ordCC+randi(4,1,2)
240     xyLim=5*[-rand(1,2); rand(1,2)]
241     dx = diff(xyLim)./nPatch./nSubP.*rand(1,2)/2
242     configPatches2(@sin,xyLim,'periodic',nPatch,ordCC ...
243         ,dx,nSubP,'EdgyInt',edgyInt,'nEdge',nEdge);

```

Check multiple fields simultaneously Set profiles to be various powers of x , ps , and store as different ‘variables’ at each point.

```

252 [ps,qs]=meshgrid(0:ordCC);
253 ps=reshape(ps,1,1,[]); qs=reshape(qs,1,1,[]);
254 cs=2*rand(size(ps))-1;
255 u0=cs.*patches.x.^ps.*patches.y.^qs;

```

Then evaluate the interpolation.

```
261 ui=patchEdgeInt2(u0(:));
```

The interior patches should have zero error. Appear to need error tolerance of 10^{-8} because of the size of the domain and the high order of interpolation.

```

269 I=ordCC/2+1:nPatch(1)-ordCC/2;
270 J=ordCC/2+1:nPatch(2)-ordCC/2;
271 error=ui(:,:, :, :, I, J)-u0(:,:, :, :, I, J);
272 assert(all(~isnan(error(:))), 'found nans in the error!')
273 hist(log10(abs(error(abs(error)>1e-20))), -20:-7)
274 xlabel('log10 error'), pause(0.3)%%
275 normError=norm(error(:))
276 assert(normError<5e-9 ...
277     , 'failed finite stencil interpolation')
278 disp('*** This finite stencil test passed')

```

End the for-loops over various parameters.

```

285 end %for realisations
286 disp('***** Passed all standard polynomial interpolation')

```

4.13.2.4 Finished

If no error messages, then all OK.

```
300 disp('***** All the interpolation tests successful')
```

5 Patches in 3D space

5.1 configPatches3(): configures spatial patches in 3D

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Makes the struct `patches` for use by the patch/gap-tooth time derivative/step function `patchSys3()`, and possibly other patch functions. [Sections 5.1.1](#) and [5.4](#) list examples of its use.

```
20 function patches = configPatches3(fun,Xlim,Dom ...
21     ,nPatch,ordCC,dx,nSubP,varargin)
22 version = '2023-04-12';
```

Input If invoked with no input arguments, then executes an example of simulating a heterogeneous wave PDE—see [Section 5.1.1](#) for an example code.

- `fun` is the name of the user function, `fun(t,u,patches)` or `fun(t,u)` or `fun(t,u,patches,...)`, 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 $[Xlim(1), Xlim(2)] \times [Xlim(3), Xlim(4)] \times [Xlim(5), Xlim(6)]$. 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 left-most/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, . . . ; 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—adjusted a little when `nEdge > 1`. So either `ratio = 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 `nSubP./nEdge` must be odd integer(s) so that there is/are

centre-patch lattice planes. So for the defaults of `nEdge` = 1 and not `EdgyInt`, then `nSubP` must be odd.

- `'nEdge'`, *optional* (integer—scalar or three element), default=1, the width of face values set by interpolation at the face regions of each patch. If two elements, then respectively the width in x, y -directions. 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. Best accuracy usually obtained when the periodicity of the coefficients is a factor of `nSubP-2*nEdge` for `EdgyInt`, or a factor of $(nSubP-nEdge)/2$ for not `EdgyInt`.
 - If `nEnsem` > 1 (value immaterial), then reset `nEnsem := m_x · m_y · m_z` and construct an ensemble of all $m_x · m_y · m_z$ 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.¹

```
225 if nargout==0, global patches, end
226 patches.version = version;
```

- `.fun` is the name of the user’s function `fun(t,u,patches)` or `fun(t,u)` or `fun(t,u,patches,...)` 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 × 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) × 1 × 1 × 1 × 1 × nPatch(1) × 1 × 1` array of the regular spatial locations x_{iI} of the microscale grid points in every patch.
- `.y` (8D) is `1 × nSubP(2) × 1 × 1 × 1 × 1 × nPatch(2) × 1` array of the regular spatial locations y_{jJ} of the microscale grid points in every patch.
- `.z` (8D) is `1 × 1 × nSubP(3) × 1 × 1 × 1 × 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` 1×3 , is the width of face values set by interpolation at the face regions of each patch, in the x, y, z -directions respectively.
- `.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

¹ When using `spmd` parallel computing, it is generally best to avoid global variables, and so instead prefer using an explicit output variable.

- 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.

5.1.1 If no arguments, then execute an example

```
315 if nargin==0
316 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.

```
334 mPeriod = [2 2 2];
335 cHetr = exp(0.9*randn([mPeriod 3]));
336 cHetr = cHetr*mean(1./cHetr(:))
```

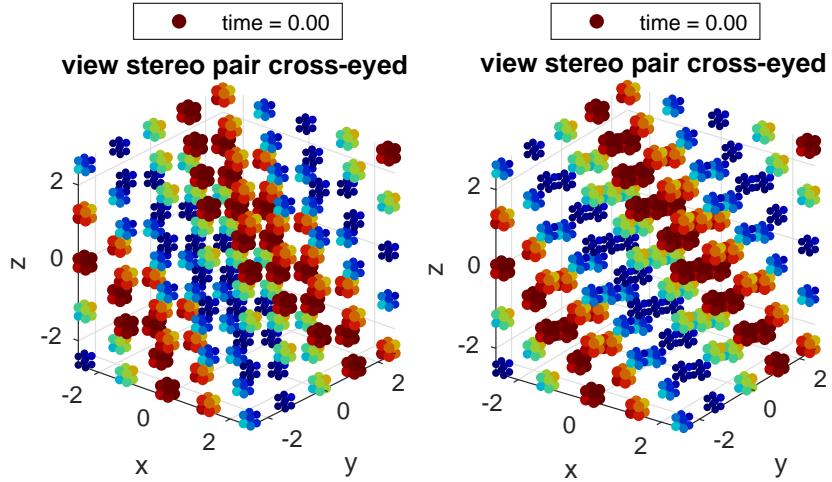
Establish global patch data struct to interface with a function coding a nonlinear 'diffusion' PDE: to be solved on $[-\pi, \pi]^3$ -periodic domain, with 5^3 patches, spectral interpolation (0) couples the patches, each patch with micro-grid spacing 0.22 (relatively large for visualisation), and with 4^3 points forming each patch.

```
348 global patches
349 patches = configPatches3(@heteroWave3, [-pi pi] ...
350 , 'periodic', 5, 0, 0.22, mPeriod+2, 'EdgyInt', true ...
351 , 'hetCoeffs', cHetr);
```

Set a wave initial state using auto-replication of the spatial grid, and as [Figure 5.1](#) shows. This wave propagates diagonally across space. Concatenate the two u, v -fields to be the two components of the fourth dimension.

```
361 u0 = 0.5+0.5*sin(patches.x+patches.y+patches.z);
362 v0 = -0.5*cos(patches.x+patches.y+patches.z)*sqrt(3);
363 uv0 = cat(4,u0,v0);
```

Figure 5.1: initial field $u(x, y, z, t)$ at time $t = 0$ of the patch scheme applied to a heterogeneous wave PDE: Figure 5.2 plots the computed field at time $t = 6$.



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 et al. 2020, Fig. 4).

```

380 disp('Simulate heterogeneous wave u_tt=div[C*grad(u)]')
381 if ~exist('OCTAVE_VERSION','builtin')
382     [ts,us] = ode23(@patchSys3,linspace(0,6),uv0(:));
383 else %disp('octave version is very slow for me')
384     lsode_options('absolute tolerance',1e-4);
385     lsode_options('relative tolerance',1e-4);
386     [ts,us] = odeOcts(@patchSys3,[0 1 2],uv0(:));
387 end

```

Animate the computed simulation to end with Figure 5.2. 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.

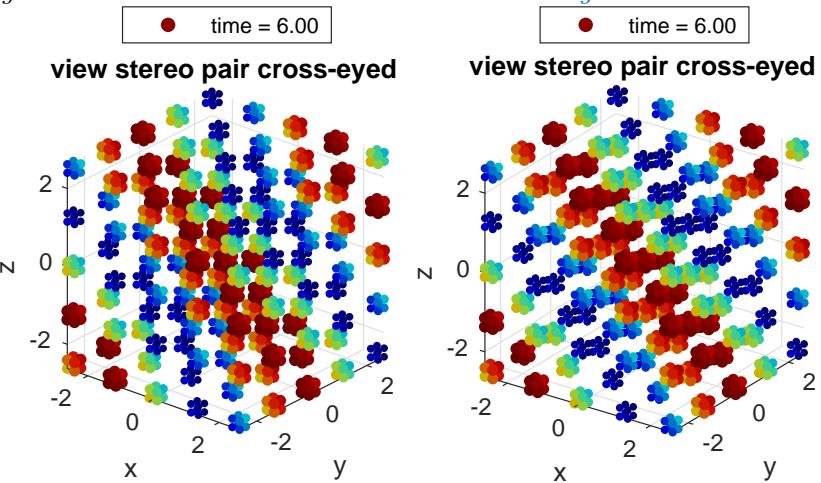
```

401 figure(1), clf, colormap(0.8*jet)
402 xs = patches.x+0*patches.y+0*patches.z;
403 ys = patches.y+0*patches.x+0*patches.z;
404 zs = patches.z+0*patches.y+0*patches.x;
405 if 1, xs([1 end],:,:)=nan;
406     xs(:,[1 end],:,:)=nan;
407     xs(:,:,1,:)=nan;
408 end;%option
409 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.

Figure 5.2: 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 5.1.



```

417 pix = @ (u) 15*abs(u)+7;
418 col = @ (u) sign(u).*abs(u);

Loop to plot at each and every time step.

424 for i = 1:length(ts)
425     uv = patchEdgeInt3(us(i,:));
426     u = uv(:,:,:,:,1,:);
427     for p=1:2
428         subplot(1,2,p)
429         if (i==1) | exist('OCTAVE_VERSION','builtin')
430             scat(p) = scatter3(xs(j),ys(j),zs(j),'filled');
431             axis equal, caxis(col([0 1])), view(45-5*p,25)
432             xlabel('$x$'), ylabel('$y$'), zlabel('$z$')
433             title('view stereo pair cross-eyed')
434         end % in matlab just update values
435         set(scat(p),'CData',col(u(j)) ...
436             , 'SizeData',pix((8+xs(j)-ys(j)+zs(j))/6+0*u(j)));
437         legend(['time = ' num2str(ts(i),'%4.2f')],'Location','north')
438     end

```

Optionally save the initial condition to graphic file for Figure 4.1, and optionally save the last plot.

```

446 if i==1,
447     ifOurCf2eps([mfilename 'ic'])
448         disp('Type space character to animate simulation')
449         pause
450     else pause(0.05)
451     end
452 end% i-loop over all times
453 ifOurCf2eps([mfilename 'fin'])

```

Upon finishing execution of the example, exit this function.

```

468   return
469   end%if no arguments

```

5.1.2 heteroWave3(): heterogeneous Waves

This function codes the lattice heterogeneous waves inside the patches. The wave PDE is

$$u_t = v, \quad v_t = \vec{\nabla}(C\vec{\nabla} \cdot u)$$

for diagonal matrix C which has microscale variations. For 8D input arrays u , x , y , and z (via edge-value interpolation of `patchSys3`, [Section 5.2](#)), computes the time derivative at each point in the interior of a patch, output in `ut`. The three 3D array of heterogeneous coefficients, c_{ijk}^x , c_{ijk}^y and c_{ijk}^z , 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.

```

26   function ut = heteroWave3(t,u,patches)
27   if nargin<3, global patches, end

```

Microscale space-steps, and interior point indices.

```

33   dx = diff(patches.x(2:3)); % x micro-scale step
34   dy = diff(patches.y(2:3)); % y micro-scale step
35   dz = diff(patches.z(2:3)); % z micro-scale step
36   i = 2:size(u,1)-1; % x interior points in a patch
37   j = 2:size(u,2)-1; % y interior points in a patch
38   k = 2:size(u,3)-1; % z interior points in a patch

```

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

```

46   ut = nan+u; % preallocate output array
47   ut(i,j,k,1,:) = u(i,j,k,2,:);
48   ut(i,j,k,2,:) ...
49   =diff(patches.cs(:,j,k,1,:).*diff(u(:,j,k,1,:),1,1)/dx^2 ...
50   +diff(patches.cs(i,:,k,2,:).*diff(u(i,:,k,1,:),1,2),1,2)/dy^2 ...
51   +diff(patches.cs(i,j,:,3,:).*diff(u(i,j,:,1,:),1,3),1,3)/dz^2;
52   end% function

```

5.1.3 Parse input arguments and defaults

```

486 p = inputParser;
487 fnValidation = @(f) isa(f, 'function_handle'); %test for fn name
488 addRequired(p,'fun',fnValidation);
489 addRequired(p,'Xlim',@isnumeric);
490 %addRequired(p,'Dom'); % too flexible
491 addRequired(p,'nPatch',@isnumeric);
492 addRequired(p,'ordCC',@isnumeric);
493 addRequired(p,'dx',@isnumeric);
494 addRequired(p,'nSubP',@isnumeric);
495 addParameter(p,'nEdge',1,@isnumeric);

```

```

496 addParameter(p,'EdgyInt',false,@islogical);
497 addParameter(p,'nEnsem',1,@isnumeric);
498 addParameter(p,'hetCoeffs',[],@isnumeric);
499 addParameter(p,'parallel',false,@islogical);
500 %addParameter(p,'nCore',1,@isnumeric); % not yet implemented
501 parse(p,fun,Xlim,nPatch,ordCC,dx,nSubP,varargin{:});

```

Set the optional parameters.

```

507 patches.nEdge = p.Results.nEdge;
508 if numel(patches.nEdge)==1
509     patches.nEdge = repmat(patches.nEdge,1,3);
510 end
511 patches.EdgyInt = p.Results.EdgyInt;
512 patches.nEnsem = p.Results.nEnsem;
513 cs = p.Results.hetCoeffs;
514 patches.parallel = p.Results.parallel;
515 %patches.nCore = p.Results.nCore;

```

Initially duplicate parameters for three space dimensions as needed.

```

523 if numel(Xlim)==2, Xlim = repmat(Xlim,1,3); end
524 if numel(nPatch)==1, nPatch = repmat(nPatch,1,3); end
525 if numel(dx)==1, dx = repmat(dx,1,3); end
526 if numel(nSubP)==1, nSubP = repmat(nSubP,1,3); end

```

Check parameters.

```

533 assert(Xlim(1)<Xlim(2) ...
534     , 'first pair of Xlim must be ordered increasing')
535 assert(Xlim(3)<Xlim(4) ...
536     , 'second pair of Xlim must be ordered increasing')
537 assert(Xlim(5)<Xlim(6) ...
538     , 'third pair of Xlim must be ordered increasing')
539 assert((mod(ordCC,2)==0)|all(patches.nEdge==1) ...
540     , 'Cannot yet have nEdge>1 and staggered patch grids')
541 assert(all(3*patches.nEdge<=nSubP) ...
542     , 'too many edge values requested')
543 assert(all(rem(nSubP,patches.nEdge)==0) ...
544     , 'nSubP must be integer multiple of nEdge')
545 if ~patches.EdgyInt, assert(all(rem(nSubP./patches.nEdge,2)==1) ...
546     , 'for non-edgyInt, nSubP./nEdge must be odd integer')
547 end
548 if (patches.nEnsem>1)&all(patches.nEdge>1)
549     warning('not yet tested when both nEnsem and nEdge non-one')
550 end
551 %if patches.nCore>1
552 %    warning('nCore>1 not yet tested in this version')
553 %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.

```

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

Default macroscale conditions are periodic with evenly spaced patches.

575 if isempty(Dom), Dom=struct('type','periodic'); end
576 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.

584 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.

597 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 bound-
aries if no bcOffset specified when needed. Do so for all three directions
independently.

605 patches.periodic=false;
606 for p=1:3
607 switch Dom.type(p,:)
608 case 'periodic'
609     patches.periodic=true;
610     if isfield(Dom,'bcOffset')
611         warning('bcOffset not available for Dom.type = periodic'), end
612         msg=' not available for Dom.type = periodic';
613         if isfield(Dom,'X'), warning(['X' msg]), end
614         if isfield(Dom,'Y'), warning(['Y' msg]), end
615         if isfield(Dom,'Z'), warning(['Z' msg]), end
616 case {'equispace','chebyshev'}
617     if ~isfield(Dom,'bcOffset'), Dom.bcOffset=zeros(2,3); end
618 % for mixed with usergiven, following should still work
619     if numel(Dom.bcOffset)==1
620         Dom.bcOffset=repmat(Dom.bcOffset,2,3); end
621     if numel(Dom.bcOffset)==3
622         Dom.bcOffset=repmat(Dom.bcOffset(:,2,1); end
623         msg=' not available for Dom.type = equispace or chebyshev';
624         if (p==1)& isfield(Dom,'X'), warning(['X' msg]), end
625         if (p==2)& isfield(Dom,'Y'), warning(['Y' msg]), end
626         if (p==3)& isfield(Dom,'Z'), warning(['Z' msg]), end
627 case 'usergiven'
628 %     if isfield(Dom,'bcOffset')
629 %         warning('bcOffset not available for usergiven Dom.type'), end
630         msg=' required for Dom.type = usergiven';

```

```

631     if p==1, assert(isfield(Dom,'X'),['X' msg]), end
632     if p==2, assert(isfield(Dom,'Y'),['Y' msg]), end
633     if p==3, assert(isfield(Dom,'Z'),['Z' msg]), end
634 otherwise
635     error([Dom.type ' is unknown Dom.type'])
636 end%switch Dom.type
637 end%for p

```

5.1.4 The code to make patches

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

```
651 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.

```

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

```

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

```

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

```

Check for staggered grid and periodic case.

```

677 if patches.stag, assert(all(mod(nPatch,2)==0), ...
678     'Require an even number of patches for staggered grid')
679 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.

```
694 for q=1:3
695 qq=2*q-1;
```

Distribution depends upon `Dom.type`:

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

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

```

709 case 'periodic'
710     Q=linspace(Xlim(qq),Xlim(qq+1),nPatch(q)+1);
711     DQ=Q(2)-Q(1);
712     Q=Q(1:nPatch(q))+diff(Q)/2;
713     pEI=patches.EdgyInt;% abbreviation

```

```

714     pnE=patches.nEdge(q);% abbreviation
715     if pre2023, dx(q) = ratio(q)*DQ/(nSubP(q)-pnE*(1+pEI))*(2-pEI);
716     else          ratio(q) = dx(q)/DQ*(nSubP(q)-pnE*(1+pEI))/(2-pEI);
717     end
718     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.

```

727 case 'equispace'
728     Q=linspace(Xlim(qq)+((nSubP(q)-1)/2-Dom.bcOffset(qq))*dx(q) ...
729                 ,Xlim(qq+1)-((nSubP(q)-1)/2-Dom.bcOffset(qq+1))*dx(q) ...
730                 ,nPatch(q));
731     DQ=diff(Q(1:2));
732     width=(1+patches.EdgyInt)/2*(nSubP(q)-1-patches.EdgyInt)*dx;
733     if DQ<width*0.999999
734         warning('too many equispace patches (double overlapping)')
735     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’.²

```

752 case 'chebyshev'
753     halfWidth=dx(q)*(nSubP(q)-1)/2;
754     Q1 = Xlim(1)+halfWidth-Dom.bcOffset(qq)*dx(q);
755     Q2 = Xlim(2)-halfWidth+Dom.bcOffset(qq+1)*dx(q);
756 %   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`.

```

765 pEI=patches.EdgyInt; % abbreviation
766 pnE=patches.nEdge(q);% abbreviation
767 width=(1+pEI)/2*(nSubP(q)-pnE*(1+pEI))*dx(q);
768 for b=0:2:nPatch(q)-2
769     DQmin=(Q2-Q1-b*width)/2*( 1-cos(pi/(nPatch(q)-b-1)) );
770     if DQmin>width, break, end
771 end%for
772 if DQmin<width*0.999999
773     warning('too many Chebyshev patches (mid-domain overlap)')
774 end%if

```

Assign the centre-patch coordinates.

```

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

```

² 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??

```
782     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.

```
791 case 'usergiven'
792   if q==1, Q = reshape(Dom.X,1,[]); end
793   if q==2, Q = reshape(Dom.Y,1,[]); end
794   if q==3, Q = reshape(Dom.Z,1,[]); end
795 end%switch Dom.type
```

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

```
802 if q==1, X=Q; end
803 if q==2, Y=Q; end
804 if q==3, Z=Q; end
805 end%for q
```

Construct the micro-grids Fourth, construct the microscale grid in each patch, centred about the given mid-points X, Y, Z . Reshape the grid to be 8D to suit dimensions (micro,Vars,Ens,macro).

```
821 xs = dx(1)*( (1:nSubP(1))-mean(1:nSubP(1)) );
822 patches.x = reshape( xs'+X ...
823                           ,nSubP(1),1,1,1,1,nPatch(1),1,1);
824 ys = dx(2)*( (1:nSubP(2))-mean(1:nSubP(2)) );
825 patches.y = reshape( ys'+Y ...
826                           ,1,nSubP(2),1,1,1,1,nPatch(2),1);
827 zs = dx(3)*( (1:nSubP(3))-mean(1:nSubP(3)) );
828 patches.z = reshape( zs'+Z ...
829                           ,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.³

```
841 if patches.periodic
842   ratio = reshape(ratio,1,3); % force to be row vector
843   patches.ratio = ratio;
844   if ordCC>0
845     [Cwtsr,Cwtsl] = patchCwts(ratio,ordCC,patches.stag);
846     patches.Cwtsr = Cwtsr; patches.Cwtsl = Cwtsl;
847   end%if
848 end%if patches.periodic
```

5.1.5 Set ensemble inter-patch communication

For EdgyInt or centre interpolation respectively,

- the right-face/centre realisations $1:nEnsem$ are to interpolate to left-face le , and

³ **ToDo:** Might sometime extend to coupling via derivative values.

- 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()`.

```
877 nE = patches.nEnsem;
878 patches.le = 1:nE; patches.ri = 1:nE;
879 patches.bo = 1:nE; patches.to = 1:nE;
880 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 than 4D, then the higher-dimensions are reshaped into the 4th dimension.

```
892 if ~isempty(cs)
893     [mx,my,mz,nc] = size(cs);
894     nx = nSubP(1); ny = nSubP(2); nz = nSubP(3);
895     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.

```
903 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.

```
913 patches.nEnsem = mx*my*mz;
914 patches.cs = nan(nx-1,ny-1,nz-1,nc,mx,my,mz);
915 for k = 1:mz
916     ks = (k:k+nz-2);
917     for j = 1:my
918         js = (j:j+ny-2);
919         for i = 1:mx
920             is = (i:i+nx-2);
921             patches.cs(:,:,:,:,i,j,k) = cs(is,js,ks,:);
922         end
923     end
924 end
925 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.

```

935      mmx=(0:mx-1)'; mmy=0:my-1; mmz=shiftdim(0:mz-1,-1);
936      le = mod(mmx+mod(nx-2,mx),mx)+1;
937      patches.le = reshape( le+mx*(mmy+my*mmz) ,[],1);
938      ri = mod(mmx-mod(nx-2,mx),mx)+1;
939      patches.ri = reshape( ri+mx*(mmy+my*mmz) ,[],1);
940      bo = mod(mmy+mod(ny-2,my),my)+1;
941      patches.bo = reshape( 1+mmx+mx*(bo-1+my*mmz) ,[],1);
942      to = mod(mmy-mod(ny-2,my),my)+1;
943      patches.to = reshape( 1+mmx+mx*(to-1+my*mmz) ,[],1);
944      ba = mod(mmz+mod(nz-2,mz),mz)+1;
945      patches.ba = reshape( 1+mmx+mx*(mmy+my*(ba-1)) ,[],1);
946      fr = mod(mmz-mod(nz-2,mz),mz)+1;
947      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.  

4  

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

End the two if-statements.  

964  end%if-else nEnsem>1
965 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.*⁵

```

984 if patches.parallel
985     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.

```

994 [~,pari]=max(nPatch+0.01*(1:3));
995 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.

⁴ **ToDo:** Need to justify this and the arbitrary threshold more carefully??

⁵ If subsequently outside `spmd`, then one must use functions like `getfield(patches{1}, 'a')`.

```
1005     switch pari
1006         case 1, patches.x=codistributed(patches.x,patches.codist);
1007         case 2, patches.y=codistributed(patches.y,patches.codist);
1008         case 3, patches.z=codistributed(patches.z,patches.codist);
1009     otherwise
1010         error('should never have bad index for parallel distribution')
1011     end%switch
1012 end%spmd
```

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

```
1020 else% not parallel
1021     if isfield(patches,'codist'), rmfield(patches,'codist'); end
1022 end%if-parallel
```

Fin

```
1031 end% function
```

5.2 patchSys3(): interface 3D space to time integrators

To simulate in time with 3D spatial patches we often need to interface a users time derivative function with time integration routines such as `ode23` or `PIRK2`. This function provides an interface. Communicate patch-design variables (Section 5.1) either via the global struct `patches` or via an optional third argument. `patches` is required for the parallel computing of `spmd`, or if parameters are to be passed though to the user microscale function.

```
23 function dudt = patchSys3(t,u,patches,varargin)
24 if nargin<3, global patches, end
```

Input

- `u` is a vector/array of length $\text{prod}(\text{nSubP}) \cdot \text{nVars} \cdot \text{nEnsem} \cdot \text{prod}(\text{nPatch})$ where there are `nVars` · `nEnsem` field values at each of the points in the $\text{nSubP}(1) \times \text{nSubP}(2) \times \text{nSubP}(3) \times \text{nPatch}(1) \times \text{nPatch}(2) \times \text{nPatch}(3)$ spatial grid.
- `t` is the current time to be passed to the user's time derivative function.
- `patches` a struct set by `configPatches3()` with the following information used here.
 - `.fun` is the name of the user's function `fun(t,u,patches,...)` that computes the time derivatives on the patchy lattice. The array `u` has size $\text{nSubP}(1) \times \text{nSubP}(2) \times \text{nSubP}(3) \times \text{nVars} \times \text{nEnsem} \times \text{nPatch}(1) \times \text{nPatch}(2) \times \text{nPatch}(3)$. Time derivatives must be computed into the same sized array, although herein the patch edge-values are overwritten by zeros.
 - `.x` is $\text{nSubP}(1) \times 1 \times 1 \times 1 \times \text{nPatch}(1) \times 1 \times 1$ array of the spatial locations x_i of the microscale (i, j, k) -grid points in every patch. Currently it *must* be an equi-spaced lattice on both macro- and microscales.
 - `.y` is similarly $1 \times \text{nSubP}(2) \times 1 \times 1 \times 1 \times \text{nPatch}(2) \times 1$ array of the spatial locations y_j of the microscale (i, j, k) -grid points in every patch. Currently it *must* be an equi-spaced lattice on both macro- and microscales.
 - `.z` is similarly $1 \times 1 \times \text{nSubP}(3) \times 1 \times 1 \times 1 \times \text{nPatch}(3)$ array of the spatial locations z_k of the microscale (i, j, k) -grid points in every patch. Currently it *must* be an equi-spaced lattice on both macro- and microscales.
- `varargin`, optional, is arbitrary list of parameters to be passed onto the users time-derivative function as specified in `configPatches3`.

Output

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

Sets the edge-face values from macroscale interpolation of centre-patch values, and if necessary, reshapes the fields `u` as a 8D-array. [Section 5.3](#) describes `patchEdgeInt3()`.

```
104 sizeu = size(u);
105 u = patchEdgeInt3(u,patches);
```

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

```
116 dudt = patches.fun(t,u,patches,varargin{:});
117 m = patches.nEdge(1);
118 dudt([1:m end-m+1:end],:,:,:,:) = 0;
119 m = patches.nEdge(2);
120 dudt(:,:,1:m end-m+1:end,:,:) = 0;
121 m = patches.nEdge(3);
122 dudt(:,:,1:m end-m+1:end,:,:) = 0;
123 dudt = reshape(dudt,sizeu);
```

Fin.

5.3 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 et al. 2014, Bunder et al. 2021), or patch next-to-face values which appears better (Bunder et al. 2020). This function is primarily used by patchSys3() but is also useful for user graphics.⁶

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

```
27 function u = patchEdgeInt3(u,patches)
28 if nargin<2, global patches, end
```

Input

- **u** is a vector/array of length $\text{prod}(\text{nSubP}) \cdot \text{nVars} \cdot \text{nEnsem} \cdot \text{prod}(\text{nPatch})$ 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 $\text{nSubP1} \times 1 \times 1 \times 1 \times 1 \times \text{nPatch1} \times 1 \times 1$ 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 $1 \times \text{nSubP2} \times 1 \times 1 \times 1 \times 1 \times \text{nPatch2} \times 1$ 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 $1 \times 1 \times \text{nSubP3} \times 1 \times 1 \times 1 \times \text{nPatch3}$ 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 $\{0, 2, 4, \dots\}$
 - **.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.

⁶ Script `patchEdgeInt3test.m` verifies this code.

- `.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).
- `.nEdge`, three elements, the width of edge values set by interpolation at the x, y, z -face regions, respectively, of each patch (default is one all x, y, z -faces).
- `.nEnsem` the number of realisations in the ensemble.
- `.parallel` whether serial or parallel.

Output

- `u` is 8D array, $n_{SubP1} \cdot n_{SubP2} \cdot n_{SubP3} \cdot n_{Vars} \cdot n_{Ensem} \cdot n_{Patch1} \cdot n_{Patch2} \cdot n_{Patch3}$, 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.

```

129     if max(abs(imag(u(:))))<1e-9*max(abs(u(:)))
130         uclean=@(u) real(u);
131     else uclean=@(u) u;
132     end

```

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

```

140 [~,~,nz,~,~,~,~,Nz] = size(patches.z);
141 [~,ny,~,~,~,~,Ny,~] = size(patches.y);
142 [nx,~,~,~,~,Nx,~,~] = size(patches.x);
143 nEnsem = patches.nEnsem;
144 nVars = round( numel(u)/numel(patches.x) ...
145                 /numel(patches.y)/numel(patches.z)/nEnsem );
146 assert(numel(u) == nx*ny*nz*Nx*Ny*Nz*nVars*nEnsem ...
147         , 'patchEdgeInt3: input u has wrong size for parameters')
148 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.

```

158 I=1:Nx; Ip=mod(I,Nx)+1; Im=mod(I-2,Nx)+1;
159 J=1:Ny; Jp=mod(J,Ny)+1; Jm=mod(J-2,Ny)+1;
160 K=1:Nz; Kp=mod(K,Nz)+1; Km=mod(K-2,Nz)+1;

```

Implement multiple width edges by folding Subsample x, y, z coordinates, noting it is only differences that count *and* the microgrid x, y, z spacing must be uniform.

```

170 %x = patches.x;
171 %if patches.nEdge(1)>1
172 % m = patches.nEdge(1);
173 % x = x(1:m:nx,:,:,:, :, :, :, :);
174 % nx = nx/m;
175 % u = reshape(u,m,nx,ny,nz,nVars,nEnsem,Nx,Ny,Nz);
176 % nVars = nVars*m;
177 % u = reshape( permute(u,[2:4 1 5:9]) ...
178 % ,nx,ny,nz,nVars,nEnsem,Nx,Ny,Nz);
179 %end%if patches.nEdge(1)
180 %y = patches.y;
181 %if patches.nEdge(2)>1
182 % m = patches.nEdge(2);
183 % y = y(:,1:m:ny,:,:,:, :, :, :);
184 % ny = ny/m;
185 % u = reshape(u,nx,m,ny,nz,nVars,nEnsem,Nx,Ny,Nz);
186 % nVars = nVars*m;
187 % u = reshape( permute(u,[1 3:4 2 5:9]) ...
188 % ,nx,ny,nz,nVars,nEnsem,Nx,Ny,Nz);
189 %end%if patches.nEdge(2)
190 %z = patches.z;
191 %if patches.nEdge(3)>1
192 % m = patches.nEdge(3);
193 % z = z(:,:,1:m:nz,:,:,:, :, :, :);
194 % nz = nz/m;
195 % u = reshape(u,nx,ny,m,nz,nVars,nEnsem,Nx,Ny,Nz);
196 % nVars = nVars*m;
197 % u = reshape( permute(u,[1:2 4 3 5:9]) ...
198 % ,nx,ny,nz,nVars,nEnsem,Nx,Ny,Nz);
199 %end%if patches.nEdge(3)
200 x = patches.x;
201 y = patches.y;
202 z = patches.z;
203 if mean(patches.nEdge)>1
204 mx = patches.nEdge(1);
205 my = patches.nEdge(2);
206 mz = patches.nEdge(3);
207 x = x(1:mx:nx,:,:,:, :, :, :, :);
208 y = y(:,1:my:ny,:,:,:, :, :, :);
209 z = z(:,:,1:mz:nz,:,:,:, :, :, :);
210 nx = nx/mx;
211 ny = ny/my;
212 nz = nz/mz;
213 u = reshape(u,mx,nx,my,ny,mz,nz,nVars,nEnsem,Nx,Ny,Nz);
214 nVars = nVars*mx*my*mz;
```

```

215     u = reshape( permute(u,[2:2:6 1:2:5 7:11]) ...
216                 ,nx,ny,nz,nVars,nEnsem,Nx,Ny,Nz);
217 end;%if patches.nEdge

```

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

```

226 i0 = round((nx+1)/2);
227 j0 = round((ny+1)/2);
228 k0 = round((nz+1)/2);

```

5.3.1 Periodic macroscale interpolation schemes

```
237 if patches.periodic
```

Get the size ratios of the patches in each direction.

```

243 rx = patches.ratio(1);
244 ry = patches.ratio(2);
245 rz = patches.ratio(3);

```

5.3.1.1 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.

```

256 ordCC = patches.ordCC;
257 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.

```

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

```

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

```
285 szU0=size(U); szU0=[szU0 ones(1,8-length(szU0)) ordCC];
```

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

```

295 if ~patches.parallel, dmu = zeros(szU0); % 9D
296 else dmu = zeros(szU0, patches.codist); % 9D
297 end%if patches.parallel

```

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

```

303 if patches.stag % use only odd numbered neighbours
304     error('polynomial interpolation not yet for staggered patch coupling')
305 %
306 % dmux(:, :, :, :, :, I, :, :, 1) = (Ux(:, :, :, :, :, Ip, :, :) + Ux(:, :, :, :, :, Im, :, :))/2;
307 % dmux(:, :, :, :, :, I, :, :, 2) = (Ux(:, :, :, :, :, Ip, :, :) - Ux(:, :, :, :, :, Im, :, :));
308 % Ip = Ip(Ip); Im = Im(Im); % increase shifts to \pm2
309 % dmuy(:, :, :, :, :, J, :, 1) = (Ux(:, :, :, :, :, Jp, :) + Ux(:, :, :, :, :, Jm, :))/2;
310 % dmuy(:, :, :, :, :, J, :, 2) = (Ux(:, :, :, :, :, Jp, :) - Ux(:, :, :, :, :, Jm, :)); %
311 % Jp = Jp(Jp); Jm = Jm(Jm); % increase shifts to \pm2
312 % dmuz(:, :, :, :, :, K, 1) = (Ux(:, :, :, :, :, Kp, :) + Ux(:, :, :, :, :, Km, :))/2;
313 % dmuz(:, :, :, :, :, K, 2) = (Ux(:, :, :, :, :, Kp, :) - Ux(:, :, :, :, :, Km, :)); %
314 % Kp = Kp(Kp); Km = Km(Km); % increase shifts to \pm2
315 else %disp('starting standard interpolation')
316     dmu(:, :, :, :, :, I, :, :, 1) = (U(:, :, :, :, :, Ip, :, :) ...
317                                         - U(:, :, :, :, :, Im, :, :))/2; %\mu\delta
318     dmu(:, :, :, :, :, I, :, :, 2) = (U(:, :, :, :, :, Ip, :, :) ...
319                                         - 2*U(:, :, :, :, :, I, :, :)) + U(:, :, :, :, :, Im, :, :)); %\delta^2
320 end% if stag

```

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

```

326 for k = 3:ordCC
327     dmu(:, :, :, :, :, I, :, :, k) = dmu(:, :, :, :, :, Ip, :, :, k-2) ...
328         - 2*dmu(:, :, :, :, :, I, :, :, k-2) + dmu(:, :, :, :, :, Im, :, :, k-2);
329 end

```

Interpolate macro-values to be Dirichlet face values for each patch ([Roberts & Kevrekidis 2007](#), [Bunder et al. 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`.

```

345 k=1+patches.EdgyInt; % use centre or two faces
346 u(nx, 2:(ny-1), 2:(nz-1), :, patches.ri, I, :, :) ...
347     = U(1, :, :, :, :, :, :)*(1-patches.stag) ...
348     + sum( shiftdim(patches.Cwtsr(:, 1), -8).*dmu(1, :, :, :, :, :, :, :, :, :), 9);
349 u(1, 2:(ny-1), 2:(nz-1), :, patches.le, I, :, :) ...
350     = U(k, :, :, :, :, :, :)*(1-patches.stag) ...
351     + 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.

```

363 if patches.EdgyInt % interpolate next-to-face values
364   U = u(:,[2 ny-1],2:(nz-1),:,:,I,J,K);
365 else % interpolate centre-cross values
366   U = u(:,j0,2:(nz-1),:,:,I,J,K);
367 end;%if patches.EdgyInt

```

Adjoin extra dimension for the array of differences.

```

373 szU0=size(U); szU0=[szU0 ones(1,8-length(szU0)) ordCC];

```

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

```

380 if ~patches.parallel, dmu = zeros(szU0); % 9D
381 else dmu = zeros(szU0,patches.codist); % 9D
382 end%if patches.parallel

```

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

```

388 if patches.stag % use only odd numbered neighbours
389   error('polynomial interpolation not yet for staggered patch coupling')
390 else %disp('starting standard interpolation')
391   dmu(:,:,(:,:,J,:1) = (U(:,:,(:,:,Jp,:)) ...
392                           -U(:,:,(:,:,Jm,:))/2; \%mu\delta
393   dmu(:,:,(:,:,J,:2) = (U(:,:,(:,:,Jp,:)) ...
394                           -2*U(:,:,(:,:,J,:)) +U(:,:,(:,:,Jm,:)); \%delta^2
395 end% if stag

```

Recursively take δ^2 .

```

401 for k = 3:ordCC
402   dmu(:,:,(:,:,J,:k) = dmu(:,:,(:,:,Jp,:k-2) ...
403   -2*dmu(:,:,(:,:,J,:k-2) +dmu(:,:,(:,:,Jm,:k-2));
404 end

```

Interpolate macro-values using the weights pre-computed by `configPatches3()`.
An ensemble of configurations may have cross-coupling.

```

412 k=1+patches.EdgyInt; % use centre or two faces
413 u(:,ny,2:(nz-1),:,patches.to,:,:J,:)
414   = U(:,1,:,:,:,,:)*(1-patches.stag) ...
415   +sum( shiftdim(patches.Cwtsr(:,2),-8).*dmu(:,1,:,:,:, :, :, :),9);
416 u(:,1,2:(nz-1),:,patches.bo,:,:J,:)
417   = U(:,k,:,:,:,,:)*(1-patches.stag) ...
418   +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.

```

429 if patches.EdgyInt % interpolate next-to-face values
430   U = u(:,:,2 nz-1),:,:,I,J,K);
431 else % interpolate centre-cross values
432   U = u(:,:,k0,:,:I,J,K);
433 end;%if patches.EdgyInt

```

Adjoin extra dimension for the array of differences.

```
439 szU0=size(U); szU0=[szU0 ones(1,8-length(szU0)) ordCC];
```

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

```
446 if ~patches.parallel, dmu = zeros(szU0); % 9D
447 else dmu = zeros(szU0,patches.codist); % 9D
448 end%if patches.parallel
```

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

```
454 if patches.stag % use only odd numbered neighbours
455 error('polynomial interpolation not yet for staggered patch coupling')
456 else %disp('starting standard interpolation')
457 dmu(:,:,(:,:,,:,K,1) = (U(:,:,(:,:,,:,Kp) ...
458 -U(:,:,(:,:,Km))/2; %\mu\delta
459 dmu(:,:,(:,:,,:,K,2) = (U(:,:,(:,:,Kp) ...
460 -2*U(:,:,(:,:,K) +U(:,:,(:,:,Km)); %\delta^2
461 end% if stag
```

Recursively take δ^2 .

```
467 for k = 3:ordCC
468 dmu(:,:,(:,:,K,k) = dmu(:,:,(:,:,Kp,k-2) ...
469 -2*dmu(:,:,(:,:,K,k-2) +dmu(:,:,(:,:,Km,k-2);
470 end
```

Interpolate macro-values using the weights pre-computed by `configPatches3()`.
An ensemble of configurations may have cross-coupling.

```
478 k=1+patches.EdgyInt; % use centre or two faces
479 u(:,:,nz,:,patches.fr,:,:K) ...
480 = U(:,:,1,:,:,:)*(1-patches.stag) ...
481 +sum( shiftdim(patches.Cwtsr(:,3),-8).*dmu(:,:,1,:,:,:,:) ,9);
482 u(:,:,1,:,:K) ...
483 = U(:,:,k,:,:,:)*(1-patches.stag) ...
484 +sum( shiftdim(patches.Cwtsl(:,3),-8).*dmu(:,:,k,:,:,:) ,9);
```

5.3.1.2 Case of spectral interpolation

Assumes the domain is macro-periodic.

```
494 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 $\mathbf{ks} = k2\pi/N$ for ‘wavenumbers’ $k = (0, 1, \dots, k_{\max}, -k_{\max}, \dots, -1)$ for odd N , and $k = (0, 1, \dots, k_{\max}, \pm(k_{\max} + 1) - k_{\max}, \dots, -1)$ 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.

```

517 if patches.stag % transform by doubling the number of fields
518 error('staggered grid not yet implemented??')
519 v=nan(size(u)); % currently to restore the shape of u
520 u=cat(3,u(:,1:2:nPatch,:),u(:,2:2:nPatch,:));
521 stagShift=reshape(0.5*[ones(nVars,1);-ones(nVars,1)],1,1,[]);
522 iV=[nVars+1:2*nVars 1:nVars]; % scatter interp to alternate field
523 r=r/2; % ratio effectively halved
524 nPatch=nPatch/2; % halve the number of patches
525 nVars=nVars*2; % double the number of fields
526 else % the values for standard spectral
527     stagShift = 0;
528     iV = 1:nVars;
529 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.

```
539 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, $k = (0, 1, \dots, k_{\max}, +k_{\max} + 1) - k_{\max}, \dots, -1)$.

```

552 kMax = floor((Nx-1)/2);
553 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`.

```

567 if ~patches.EdgyInt
568     Cm = fft( u(i0,iy,iz,:,:,:,:,:) ,[],6);
569     Cp = Cm;
570 else
571     Cm = fft( u( 2,iy,iz ,:,patches.le,:,:,:) ,[],6);
572     Cp = fft( u(nx-1,iy,iz ,:,patches.ri,:,:,:) ,[],6);
573 end%if ~patches.EdgyInt

```

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

```

580 u(nx,iy,iz,:,:,:,:)=uclean( ifft( ...
581     Cm.*exp(1i*(stagShift+kr)) ,[],6);

```

```
582 u( 1,iy,iz,:,:,:, :, :) = uclean( ifft( ...
583     Cp.*exp(1i*(stagShift-kr)) ,[],6) );
```

y-normal face values Set wavenumbers into a vector.

```
593 kMax = floor((Ny-1)/2);
594 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.

```
601 if ~patches.EdgyInt
602     Cm = fft( u(:,j0,iz,:,:,:, :, :) ,[],7);
603     Cp = Cm;
604 else
605     Cm = fft( u(:,2 ,iz ,:,patches.bo,:,:,:) ,[],7);
606     Cp = fft( u(:,ny-1,iz ,:,patches.to,:,:,:) ,[],7);
607 end%if ~patches.EdgyInt
```

Invert the Fourier transforms to complete interpolation.

```
613 u(:,ny,iz,:,:,:, :, :) = uclean( ifft( ...
614     Cm.*exp(1i*(stagShift+kr)) ,[],7) );
615 u(:, 1,iz,:,:,:, :, :) = uclean( ifft( ...
616     Cp.*exp(1i*(stagShift-kr)) ,[],7) );
```

z-normal face values Set wavenumbers into a vector.

```
626 kMax = floor((Nz-1)/2);
627 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.

```
634 if ~patches.EdgyInt
635     Cm = fft( u(:, :,k0,:,:,:, :, :) ,[],8);
636     Cp = Cm;
637 else
638     Cm = fft( u(:, :,2 ,:,patches.ba,:,:,:) ,[],8);
639     Cp = fft( u(:, :,nz-1 ,:,patches.fr,:,:,:) ,[],8);
640 end%if ~patches.EdgyInt
```

Invert the Fourier transforms to complete interpolation.

```
646 u(:, :,nz,:,:,:, :, :) = uclean( ifft( ...
647     Cm.*exp(1i*(stagShift+kr)) ,[],8) );
648 u(:, :, 1,:,:,:, :, :) = uclean( ifft( ...
649     Cp.*exp(1i*(stagShift-kr)) ,[],8) );
655 end% if ordCC>0
```

5.3.2 Non-periodic macroscale interpolation

```

666 else% patches.periodic false
667 assert(~patches.stag, ...
668 '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 \mathbf{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.

```

682 if patches.ordCC<1
683     px = Nx-1; py = Ny-1; pz = Nz-1;
684 else px = min(patches.ordCC,Nx-1);
685     py = min(patches.ordCC,Ny-1);
686     pz = min(patches.ordCC,Nz-1);
687 end
688 % interior indices of faces (ix n/a)
689 ix=2:nx-1; iy=2:ny-1; iz=2:nz-1;

```

5.3.2.1 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.⁷

```

702 F = nan(patches.EdgyInt+1,ny-2,nz-2,nVars,nEnsem,Nx,Ny,Nz,px+1);
703 if patches.EdgyInt % interpolate next-to-face values
704     F(:,:,(:,:,(:,:,1)) = u([nx-1 2],iy,iz,:,:,:,:,:);
705     X = x([nx-1 2],(:,:,(:,:,1));
706 else % interpolate mid-patch cross-patch values
707     F(:,:,(:,:,(:,:,1)) = u(i0,iy,iz,:,:,:,:,:);
708     X = x(i0,:,:,:,:,:);
709 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.

```

722 for q = 1:px
723     i = 1:Nx-q;
724     F(:,:,(:,:,i,:,:,:q+1) ...
725     = ( F(:,:,(:,:,i+1,:,:,:q)-F(:,:,(:,:,i,:,:,:q)) ...
726         ./ (X(:,:,(:,:,i+q,:,:))-X(:,:,(:,:,i,:,:)));
727 end

```

⁷ **ToDo:** Have no plans to implement core averaging as yet.

Interpolate with divided differences Now interpolate to find the face-values on left/right faces at X_{face} for every interior Y, Z .

```
736 Xface = 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.

```
747 i = max(1,min(1:Nx,Nx-ceil(px/2))-floor(px/2));
748 Uface = F(:,:,(:,:,i,:,:,:px+1);
749 for q = px:-1:1
750     Uface = F(:,:,(:,:,i,:,:,:q) ...
751         +(Xface-X(:,:,(:,:,i+q-1,:,:)).*Uface;
752 end
```

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

```
760 u(1 ,iy,iz,:,:patches.le,:,:,:) = Uface(1,:,:,:,:,:,:,:);
761 u(nx,iy,iz,:,:patches.ri,:,:,:) = Uface(2,:,:,:,:,:,:,:);
```

5.3.2.2 y -direction values

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

```
771 F = nan(nx,patches.EdgyInt+1,nz-2,nVars,nEnsem,Nx,Ny,Nz,py+1);
772 if patches.EdgyInt % interpolate next-to-face values
773     F(:,:,(:,:,1,:,:,:)) = u(:,:,ny-1 2,iz,:,:,:,:,:);
774     Y = y(:,:,ny-1 2,:,:,:,:,:,:);
775 else % interpolate mid-patch cross-patch values
776     F(:,:,(:,:,1,:,:,:)) = u(:,:,j0,iz,:,:,:,:,:);
777     Y = y(:,:,j0,:,:,:,:,:,:);
778 end%if patches.EdgyInt
```

Form tables of divided differences.

```
784 for q = 1:py
785     j = 1:Ny-q;
786     F(:,:,(:,:,j,q+1) ... 
787     = ( F(:,:,(:,:,j+1,q)-F(:,:,(:,:,j,q)) ...
788         ./(Y(:,:,(:,:,j+q,:)-Y(:,:,(:,:,j,:));
```

```
789 end
```

Interpolate to find the top/bottom faces Y_{face} for every x and interior z .

```
796 Yface = 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.

```

805     j = max(1,min(1:Ny,Ny-ceil(py/2))-floor(py/2));
806     Uface = F(:,:,(:,:,j,:,:,py+1));
807     for q = py:-1:1
808         Uface = F(:,:,(:,:,j,q)) ...
809             +(Yface-Y(:,:,(:,:,j+q-1,:))).*Uface;
810     end

```

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

```

818 u(:,:,iz,:,:,patches.bo,:,:,:) = Uface(:,:,1,:,:,:,:,:);
819 u(:,:,ny,iz,:,:,patches.to,:,:,:) = Uface(:,:,2,:,:,:,:,:);

```

5.3.2.3 z -direction values

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

```

829 F = nan(nx,ny,patches.EdgyInt+1,nVars,nEnsem,Nx,Ny,Nz,pz+1);
830 if patches.EdgyInt % interpolate next-to-face values
831     F(:,:,(:,:,1,:,:,1)) = u(:,:,,[nz-1 2],:,:,:,:);
832     Z = z(:,:,,[nz-1 2],:,:,:,:);
833 else % interpolate mid-patch cross-patch values
834     F(:,:,(:,:,k0,:,:,1,:)) = u(:,:,k0,:,:,:,:,:);
835     Z = z(:,:,k0,:,:,:,:,:);
836 end%if patches.EdgyInt

```

Form tables of divided differences.

```

842 for q = 1:pz
843     k = 1:Nz-q;
844     F(:,:,(:,:,k,q+1)) ...
845     = ( F(:,:,(:,:,k+1,q))-F(:,:,(:,:,k,q)) ...
846         ./(Z(:,:,(:,:,k+q))-Z(:,:,(:,:,k)));
847 end

```

Interpolate to find the face-values on front/back faces Z_{face} for every x, y .

```
854 Zface = 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.

```

863 k = max(1,min(1:Nz,Nz-ceil(pz/2))-floor(pz/2));
864 Uface = F(:,:,(:,:,k,pz+1));
865 for q = pz:-1:1
866     Uface = F(:,:,(:,:,k,q)) ...
867         +(Zface-Z(:,:,(:,:,k+q-1))).*Uface;
868 end

```

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

```

876 u(:,:,1,:,:patches.fr,:,:,:) = Uface(:,:,1,:,:,:,:,:);
877 u(:,:,nz,:,:patches.ba,:,:,:) = Uface(:,:,2,:,:,:,:,:);
```

5.3.2.4 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, unless testing, override their computed interpolation values with NaN.

```

889 if isfield(patches,'intTest')&&patches.intTest
890 else % usual case
891     u( 1,:,:,:, :, 1,:,:,:) = nan;
892     u(nx,:,:,:, :,Nx,:,:) = nan;
893     u(:, 1,:,:,:, :, 1,:) = nan;
894     u(:,ny,:,:,:, :,Ny,:) = nan;
895     u(:,:, 1,:,:,:, :, 1) = nan;
896     u(:,:,nz,:,:,:, :,Nz) = nan;
897 end%if
```

End of the non-periodic interpolation code.

```

904 end%if patches.periodic else
```

Unfold multiple edges No need to restore x, y, z .

```

911 if mean(patches.nEdge)>1
912     nVars = nVars/(mx*my*mz);
913     u = reshape( u ,nx,ny,nz,mx,my,mz,nVars,nEnsem,Nx,Ny,Nz);
914     nx = nx*mx;
915     ny = ny*my;
916     nz = nz*mz;
917     u = reshape( permute(u,[4 1 5 2 6 3 7:11]) ...
918                 ,nx,ny,nz,nVars,nEnsem,Nx,Ny,Nz);
919 end%if patches.nEdge
```

Fin, returning the 8D array of field values with interpolated faces.

```

927 end% function patchEdgeInt3
```

5.4 homoDiffEdgy3: computational homogenisation of a 3D diffusion via simulation on small patches

Simulate heterogeneous diffusion in 3D space on 3D patches as an example application. Then compute macroscale eigenvalues of the patch scheme applied to this heterogeneous diffusion to validate and to compare various orders of inter-patch interpolation.

This code extends to 3D the 2D code discussed in [Section 4.5](#). First 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.

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

Configure the patch scheme with some arbitrary choices of domain, patches, size ratios. Use spectral interpolation as we test other orders subsequently. In 3D we appear to get only real eigenvalues by using edgy interpolation. What happens for non-edgy interpolation is unknown.

```
42 nSubP=mPeriod+2;
43 nPatch=[5 5 5];
44 configPatches3(@heteroDiff3, [-pi pi], nan, nPatch ...
45 ,0, 0.3, nSubP, 'EdgyInt',true ...
46 , 'hetCoeffs',cHetr );
```

5.4.1 Simulate heterogeneous diffusion

Set initial conditions of a simulation as shown in [Figure 5.3](#).

```
56 global patches
57 u0 = exp(-patches.x.^2/4-patches.y.^2/2-patches.z.^2);
58 u0 = u0.*((1+0.3*rand(size(u0))));
```

Integrate using standard integrators, unevenly spaced in time to better display transients.

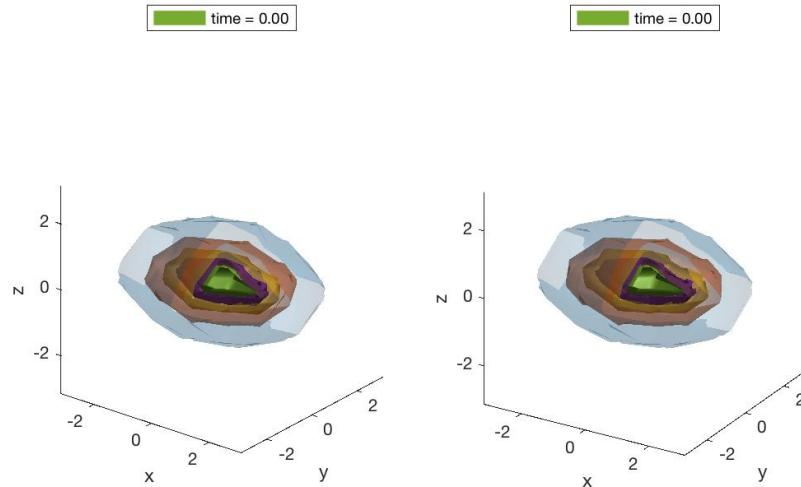
```
76 if ~exist('OCTAVE_VERSION','builtin')
77 [ts,us] = ode23(@patchSys3, 0.3*linspace(0,1,50).^2, u0(:));
78 else % octave version
79 [ts,us] = odeOcts(@patchSys3, 0.3*linspace(0,1).^2, u0(:));
80 end
```

Plot the solution as an animation over time.

```
88 figure(1), clf
89 rgb=get(gca,'defaultAxesColorOrder');
90 colormap(0.8*hsv)
```

Get spatial coordinates of patch interiors.

Figure 5.3: initial field $u(x, y, z, 0)$ of the patch scheme applied to a heterogeneous diffusion PDE. Plotted are the isosurfaces at field values $u = 0.1, 0.3, \dots, 0.9$, with the front quadrant omitted so you can see inside. Figure 5.4 plots the isosurfaces of the computed field at time $t = 0.3$.



```

96 x = reshape( patches.x([2:end-1],:,:, :) ,[],1);
97 y = reshape( patches.y(:,[2:end-1],:,:, :) ,[],1);
98 z = reshape( patches.z(:,:, [2:end-1],:) ,[],1);

```

For every time step draw the surface and pause for a short display.

```
105 for i = 1:length(ts)
```

Get the row vector of data, form into a 6D array, then omit patch faces, and reshape to suit the isosurface function. We do not use interpolation to get face values as the interpolation omits the corner edges and so breaks up the isosurfaces.

```

115 u = reshape( us(i,:), [nSubP nPatch]);
116 u = u([2:end-1],[2:end-1],[2:end-1],:,:,:,:);
117 u = reshape( permute(u,[1 4 2 5 3 6]) ...
118 , [numel(x) numel(y) numel(z)]);

```

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

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

The `isosurface` function requires us to transpose x and y .

```
131 v = permute(u,[2 1 3]);
```

Draw cross-eyed stereo view of some isosurfaces.

```

137 clf;
138 for p=1:2
139 subplot(1,2,p)
140 for iso=5:-1:1
141 isov=(iso-0.5)/5;
142 hsurf(iso) = patch(isosurface(x,y,z,v, isov));
143 isonormals(x,y,z,v,hsurf(iso))
144 set(hsurf(iso) , 'FaceColor',rgb(iso,:)) ...
145 , 'EdgeColor','none' ...
146 , 'FaceAlpha',iso/5);
147 hold on
148 end
149 axis equal, view(45-7*p,25)
150 axis(pi*[-1 1 -1 1 -1 1])
151 xlabel('$x$'), ylabel('$y$'), zlabel('$z$')
152 legend(['time = ' num2str(ts(i),'%4.2f')],'Location','north')
153 camlight, lighting gouraud
154 hold off
155 end% each p
156 if i==1 % pause for the viewer
157 makeJpeg=false;
158 if makeJpeg, print(['Figs/' mfilename 't0'], '-djpeg'), end
159 disp('Press any key to start animation of isosurfaces')
160 pause
161 else pause(0.05)
162 end
163
164 end%for over time
165 if makeJpeg, print(['Figs/' mfilename 'tFin'], '-djpeg'), end

```

Finish the animation loop, and optionally output the isosurfaces of the final field, [Figure 5.4](#).

5.4.2 Compute Jacobian and its spectrum

Let's explore the Jacobian dynamics for a range of orders of interpolation, all for the same random patch design and heterogeneity. Except here use a small ratio as we do not plot and then the scale separation is clearest.

```

195 ratio = 0.025*(1+rand(1,3))
196 nSubP=randi([3 5],1,3)
197 nPatch=[3 3 3]
198 nEnsem = prod(mPeriod) % or just set one

```

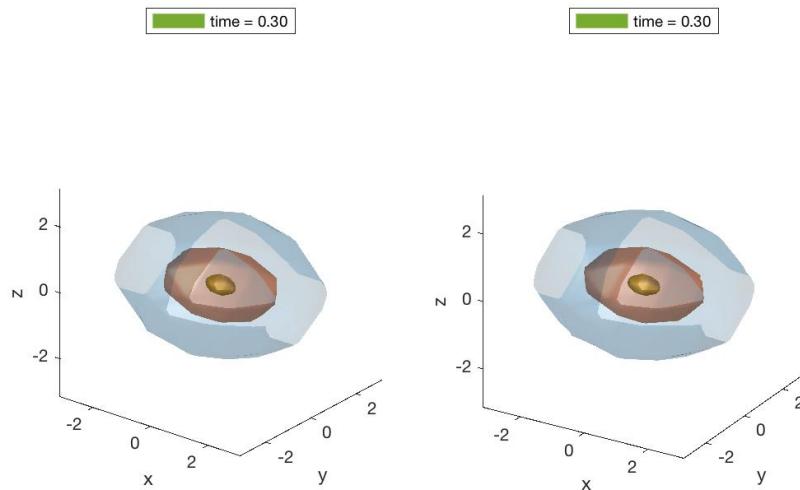
Find which elements of the 8D array are interior micro-grid points and hence correspond to dynamical variables.

```

205 u0 = zeros([nSubP,1,nEnsem,nPatch]);
206 u0([1 end],:,:,:)=nan;
207 u0(:,:,1,:)=nan;
208 u0(:,:,1,:)=nan;

```

Figure 5.4: final field $u(x, y, z, 0.3)$ of the patch scheme applied to a heterogeneous diffusion PDE. Plotted are the isosurfaces at field values $u = 0.1, 0.3, \dots, 0.9$, with the front quadrant omitted so you can see inside.



```

209 i = find(~isnan(u0));
210 sizeJacobian = length(i)
211 assert(sizeJacobian<4000 ...
212 , 'Jacobian is too big to quickly generate and analyse')

Store this many eigenvalues in array across different orders of interpolation.

219 nLeadEvals=prod(nPatch)+max(nPatch);
220 leadingEvals=[];

Evaluate eigenvalues for spectral as the base case for polynomial interpolation
of order 2, 4, ....

228 maxords=6;
229 for ord=0:2:maxords
    ord=ord

Configure with same heterogeneity.

236 configPatches3(@heteroDiff3, [-pi pi], nan, nPatch ...
237 , ord, ratio, nSubP, 'EdgyInt', true, 'nEnsem', nEnsem ...
238 , 'hetCoeffs', cHetr);

```

Construct the Jacobian of the scheme as the matrix of the linear transformation, obtained by transforming the standard unit vectors.

```

246 jac = nan(length(i));
247 for j = 1:length(i)

```

```

248      u = u0(:)+(i(j)==(1:numel(u0))');
249      tmp = patchSys3(0,u);
250      jac(:,j) = tmp(i);
251  end

```

Test for symmetry, with error if we know it should be symmetric.

```

258      notSymmetric=norm(jac-jac')
259  %    if notSymmetric>1e-7, spy(abs(jac-jac')>1e-7), end%??
260      assert(notSymmetric<1e-7,'failed symmetry')

```

Find all the eigenvalues (as `eigs` is unreliable), and put eigenvalues in a vector.

```

267      [evecs,evals] = eig((jac+jac')/2,'vector');
268      biggestImag=max(abs(imag(evals)));
269      if biggestImag>0, biggestImag=biggestImag, end

```

Sort eigenvalues on their real-part with most positive first, and most negative last. Store the leading eigenvalues in `egs`, and write out when computed all orders. The number of zero eigenvalues, `nZeroEv`, gives the number of decoupled systems in this patch configuration.

```

279      [~,k] = sort(-real(evals));
280      evals=evals(k); evecs=evecs(:,k);
281      if ord==0, nZeroEv=sum(abs(evals(:))<1e-5), end
282      if ord==0, evec0=evecs(:,1:nZeroEv*nLeadEvals);
283      else % find evec closest to that of each leading spectral
284          [~,k]=max(abs(evecs'*evec0));
285          evals=evals(k); % re-sort in corresponding order
286      end
287      leadingEvals=[leadingEvals evals(nZeroEv*(1:nLeadEvals))];
288  end
289  disp('    spectral    quadratic    quartic    sixth-order ...')
290  leadingEvals=leadingEvals

```

5.4.3 `heteroDiff3()`: heterogeneous diffusion

This function codes the lattice heterogeneous diffusion inside the patches. For 8D input array `u` (via edge-value interpolation of `patchEdgeInt3`, such as by `patchSys3`, [Section 5.2](#)), computes the time derivative ([3.1](#)) at each point in the interior of a patch, output in `ut`. The three 3D array of diffusivities, c_{ijk}^x , c_{ijk}^y and c_{ijk}^z , have previously been stored in `patches.cs` (4+D).

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

```

23  function ut = heteroDiff3(t,u,patches)
24      if nargin<3, global patches, end
25
26      Microscale space-steps. Q: is using i,j,k slower than 2:end-1??
27
28      dx = diff(patches.x(2:3)); % x micro-scale step
29      dy = diff(patches.y(2:3)); % y micro-scale step

```

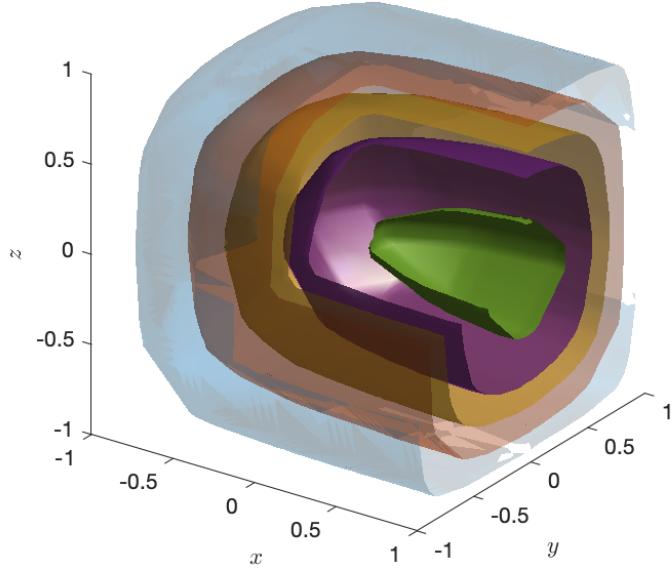
```
33     dz = diff(patches.z(2:3)); % z micro-scale step
34     i = 2:size(u,1)-1; % x interior points in a patch
35     j = 2:size(u,2)-1; % y interior points in a patch
36     k = 2:size(u,3)-1; % z interior points in a patch
```

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

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

Fin.

Figure 5.5: 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 5.5). The small patches are equispaced in space.



5.5 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 5.5 shows five isosurfaces of the 3D solution field.

Clear variables, and establish globals.

```

33 clear all
34 global patches
35 %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.

```

46 mPeriod = randi([2 3],1,3)
47 cDiff = exp(0.3*randn([mPeriod 3]));
48 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.

```

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

```

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

```

73 patches.fu = 10*exp(-patches.x.^2-patches.y.^2-patches.z.^2);
74 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.

```

87 u0 = zeros([nSubP,1,1,nPatch,nPatch,nPatch]);
88 u0([1 end],:,:, :) = nan;
89 u0(:,[1 end],:,:) = nan;
90 u0(:,:, [1 end],:) = nan;
91 patches.i = find(~isnan(u0));
92 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 3.19).

```

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

```

Store the solution into the patches, and give magnitudes.

```

112 u0(patches.i) = uSoln;
113 u0 = patchEdgeInt3(u0);

```

Plot isosurfaces of the solution

```

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

```

Reshape spatial coordinates of patches.

```

129 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.

```

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

```

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

```

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

```

Draw some isosurfaces.

```

151 clf;
152 for iso=5:-1:1
153     isov=(iso-0.5)/5*(maxu-minu)+minu;
154     hsurf(iso) = patch(isosurface(x,y,z,u, isov));
155     isonormals(x,y,z,u,hsurf(iso))
156     set(hsurf(iso) , 'FaceColor',rgb(iso,:)
157         , 'EdgeColor','none' , 'FaceAlpha',iso/5);
158     hold on
159 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 if OurCf2eps(mfilename) %optionally save plot
165 if exist('OurCf2eps') && OurCf2eps, print('-dpng',[Figs/' mfilename]), end

```

5.5.1 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`, Section 5.2), computes the time derivative at each point in the interior of a patch, output in ut . The three 3D array of diffusivities, c_{ijk}^x , c_{ijk}^y and c_{ijk}^z , 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; % z 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,:,:,:,:,:)=u(end-1,:,:,:,:,:); %right face of rightmost

```

```
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.codist)`

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

5.6 heteroDispersiveWave3: heterogeneous Dispersive Waves from 4th order PDE

This uses small spatial patches to simulate heterogeneous dispersive waves in 3D. The wave equation for $u(x, y, z, t)$ is the fourth-order in space PDE

$$u_{tt} = -\nabla^2(C\nabla^2u)$$

for microscale variations in scalar $C(x, y, z)$.

Initialise some Matlab aspects.

```
21 clear all
22 cMap=jet(64); cMap=0.8*cMap(7:end-7,:); % set colormap
23 basename = [num2str(floor(1e5*rem(now,1))) mfilename]
24 %global OurCf2eps, OurCf2eps=true %optional to save plots
```

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.

```
34 mPeriod = [2 2 2];
35 cHetr = exp(0.9*randn(mPeriod));
36 cHetr = cHetr*mean(1./cHetr(:))
```

Establish global patch data struct to interface with a function coding a fourth-order heterogeneous wave 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 6^3 points forming each patch. (Six because two edge layers on each of two faces, and two interior points for the PDE.)

```
50 global patches
51 patches = configPatches3(@heteroDispWave3, [-pi pi] ...
52 , 'periodic', 5, 0, 0.22, mPeriod+4 , 'EdgyInt', true ...
53 , 'hetCoeffs', cHetr , 'nEdge', 2);
```

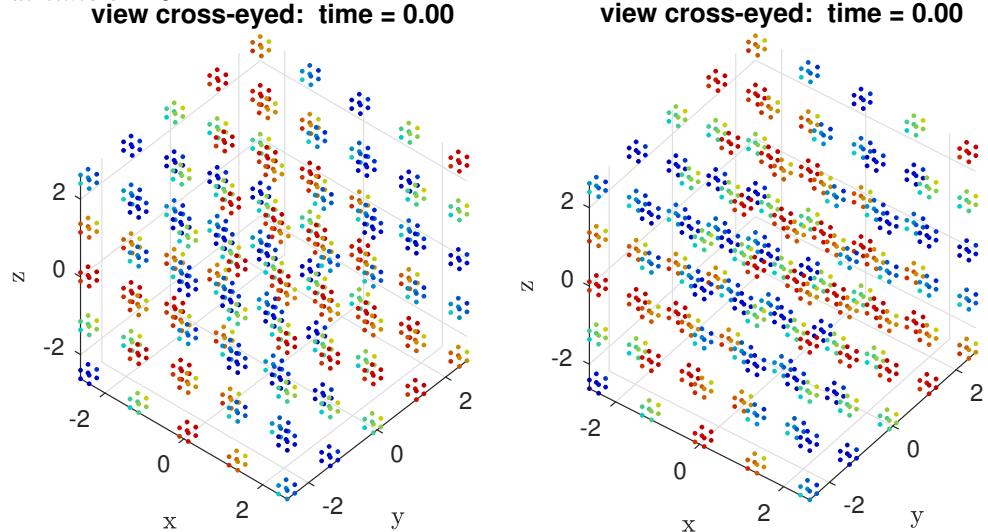
Set a wave initial state using auto-replication of the spatial grid, and as [Figure 5.6](#) shows. This wave propagates diagonally across space. Concatenate the two u, v -fields to be the two components of the fourth dimension.

```
64 u0 = 0.5+0.5*sin(patches.x+patches.y+patches.z);
65 v0 = -0.5*cos(patches.x+patches.y+patches.z)*3;
66 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 et al. 2020](#), Fig. 4).

```
83 disp('Simulate heterogeneous wave u_tt=delsq[C*delsq(u)]')
84 tic
85 [ts,us] = ode23(@patchSys3,linspace(0,6),uv0(:));
86 simulateTime=toc
```

Figure 5.6: initial field $u(x, y, z, t)$ at time $t = 0$ of the patch scheme applied to a heterogeneous dispersive wave PDE: [Figure 5.7](#) plots the computed field at time $t = 6$.



Animate the computed simulation to end with [Figure 5.7](#). 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.

```

100 %
101 figure(1), clf, colormap(cMap)
102 xs = patches.x+0*patches.y+0*patches.z;
103 ys = patches.y+0*patches.x+0*patches.z;
104 zs = patches.z+0*patches.y+0*patches.x;
105 if 1, xs([1:2 end-1:end],:,:, :)=nan;
106     xs(:,[1:2 end-1:end],:,:, :)=nan;
107     xs(:,:, [1:2 end-1:end],:)=nan;
108 end;%option
109 j=find(~isnan(xs));

```

In the scatter plot, `col()` maps the u -data values to the colour of the dots.

```
116 col = @ (u) sign(u).*abs(u);
```

Loop to plot at each and every time step.

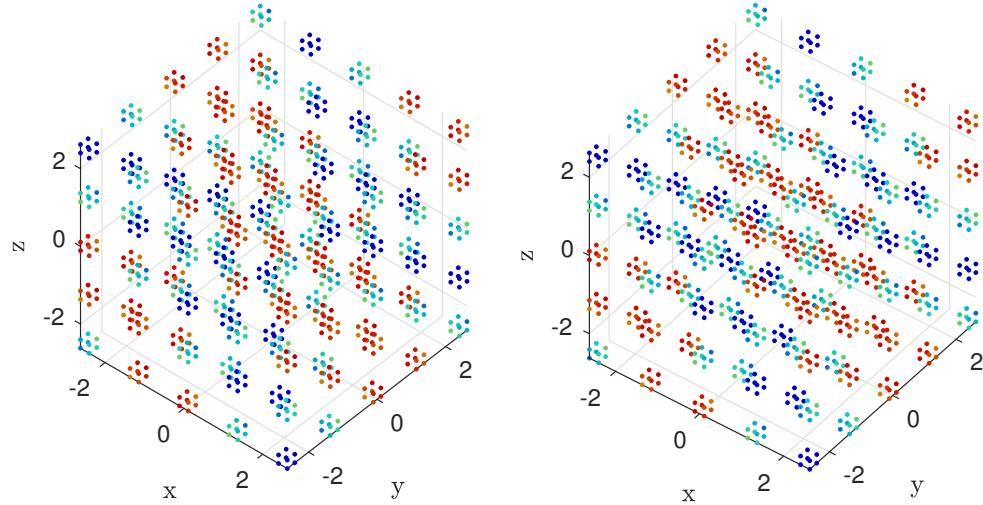
```

122 for i = 1:length(ts)
123     uv = patchEdgeInt3(us(i,:));
124     u = uv(:,:, :, 1,:);
125     for p=1:2
126         subplot(1,2,p)
127         if (i==1)
128             scat(p) = scatter3(xs(j),ys(j),zs(j),'.');

```

Figure 5.7: field $u(x, y, z, t)$ at time $t = 6$ of the patch scheme applied to the heterogeneous dispersive wave PDE with initial condition in Figure 5.6.

view cross-eyed: time = 6.00 **view cross-eyed: time = 6.00**



```

129      axis equal, caxis(col([0 1])), view(45-4*p,42)
130      xlabel('$x$'), ylabel('$y$'), zlabel('$z$')
131    end
132    title(['view cross-eyed: time = ' num2str(ts(i),'%4.2f')])
133    set( scat(p),'CData',col(u(j)) );
134  end

```

Optionally save the initial condition to graphic file for Figure 5.6, and optionally save the last plot.

```

142  if i==1,
143    ifOurCf2eps([basename 'ic'])
144      disp('Type space character to animate simulation')
145      pause
146    else pause(0.1)
147    end
148  end% i-loop over all times
149  ifOurCf2eps([basename 'fin'])

```

5.6.1 heteroDispWave3(): PDE function of 4th-order heterogeneous dispersive waves

This function codes the lattice heterogeneous waves inside the patches. The wave PDE for $u(x, y, z, t)$ and ‘velocity’ $v(x, y, z, t)$ is

$$u_t = v, \quad v_t = -\nabla^2(C\nabla^2 u)$$

for microscale variations in scalar $C(x, y, z)$. For 8D input arrays \mathbf{u} , \mathbf{x} , \mathbf{y} , and \mathbf{z} (via edge-value interpolation of `patchSys3`, Section 5.2), computes the time derivative at each point in the interior of a patch, output in \mathbf{ut} . The 3D array of heterogeneous coefficients, C_{ijk} , c_{ijk}^y and c_{ijk}^z , have been stored in `patches.cs` (3D).

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

```

187 function ut = heteroDispWave3(t,u,patches)
188     if nargin<3, global patches, end
190
191     Micro-grid space steps.
192
193     dx = diff(patches.x(2:3));
194     dy = diff(patches.y(2:3));
195     dz = diff(patches.z(2:3));

```

First, compute $C\nabla^2 u$ into say u , using indices for all but extreme micro-grid points. We use a single colon to represent the last four array dimensions because the result arrays are already dimensioned.

```

200 I = 2:size(u,1)-1; J = 2:size(u,2)-1; K = 2:size(u,3)-1;
201 u(I,J,K,1,:) = patches.cs(I,J,K,1,:).*(
202     diff(u(:,J,K,1,:),2,1)/dx^2 ...
203     +diff(u(I,:,:K,1,:),2,2)/dy^2 +diff(u(I,J,:,:1,:),2,3)/dz^2 );

```

Reserve storage, set lowercase indices to non-edge interior, and then assign interior patch values to the heterogeneous diffusion time derivatives.

```

210 ut = nan+u; % preallocate output array
211 i = I(2:end-1); j = J(2:end-1); k = K(2:end-1);
212 ut(i,j,k,1,:) = u(i,j,k,2,:); % du/dt=v
213 % dv/dt=delta^2 of above C*delta^2
214 ut(i,j,k,2,:) = -( diff(u(I,j,k,1,:),2,1)/dx^2 ...
215     +diff(u(i,J,k,1,:),2,2)/dy^2 +diff(u(i,j,K,1,:),2,3)/dz^2 );
216 end% function

```

5.6.2 patchEdgeInt3test: tests 3D patch coupling

A script to test the spectral, finite-order, and divided difference, polynomial interpolation of function `patchEdgeInt3()`. Tests one or several variables, normal grids, and also tests centre and edge interpolation. But does not yet test staggered grids, core averaging, etc as they are not yet implemented.

Start by establishing global data struct for the range of various cases. Choose a number of realisations for every type, but beware that some realisations take several minutes.

```

21 clear all, close all
22 global patches
23 nRealise = 10

```

5.6.2.1 Check divided difference interpolation

```

36 fprintf('\n\n**** Check divided difference interpolation\n')
37 pause(1)

```

Check over various types and orders of interpolation, numbers of patches, random domain lengths, random ratios, and randomised distribution of patches. (The `@sin` is a dummy.)

```

46 maxErrors=[];
47 for realisation = 1:nRealise
48     nEdge = randi(3,1,3)% =1,2, or 3
49     edgyInt = (rand>0.5)
50     Lx = 1+3*rand; Ly = 1+3*rand; Lz = 1+3*rand;
51     xyzLim = [0 Lx 0 Ly 0 Lz]-[rand*[1 1] rand*[1 1] rand*[1 1]]
52     nSubP = nEdge.*((2-edgyInt)*randi(2,1,3)+1+edgyInt)
53     ordCC = 2*randi(3)
54     nPatch = ordCC+randi(4,1,3)
55     dx = [Lx Ly Lz]./nPatch./nSubP.*rand(1,3)/2
56     configPatches3(@sin,xyzLim,'equispace',nPatch,ordCC ...
57         ,dx,nSubP,'EdgyInt',edgyInt,'nEdge',nEdge);

```

Second, displace patches to a random non-uniform spacing.

```

63 Hx = diff(patches.x(1,1,1,:,:,:1:2,1,1));
64 patches.x = patches.x+0.8*Hx*(rand(1,1,1,1,1,nPatch(1),1,1)-0.5);
65 Hx = squeeze( diff(patches.x(1,1,1,:,:,:,1,1)) );% for information only
66 Hy = diff(patches.y(1,1,1,:,:,:,1,1:2,1));
67 patches.y = patches.y+0.8*Hy*(rand(1,1,1,1,1,1,nPatch(2),1)-0.5);
68 Hy = squeeze( diff(patches.y(1,1,1,:,:,:,1,:1)) );% for information only
69 Hz = diff(patches.z(1,1,1,:,:,:,1,1:2));
70 patches.z = patches.z+0.8*Hz*(rand(1,1,1,1,1,1,nPatch(3))-0.5);
71 Hz = squeeze( diff(patches.z(1,1,1,:,:,:,1,1,:)) );% for information only

```

Check multiple fields simultaneously Set profiles to be various powers of x , y and z , **ps**, **qs** and **rs**, and store as different ‘variables’ at each point. First, limit the order of test polynomials by the order of interpolation and by the number of patches.

```

85 ox=min(ordCC,nPatch(1)-1);
86 oy=min(ordCC,nPatch(2)-1);
87 oz=min(ordCC,nPatch(3)-1);
88 [ps,qs,rs]=ndgrid(0:ox,0:oy,0:oz);
89 ps=reshape(ps,1,1,1,[ ]);
90 qs=reshape(qs,1,1,1,[ ]);
91 rs=reshape(rs,1,1,1,[ ]);
92 cs=2*rand(size(ps))-1;
93 u0=cs.*patches.x.^ps.*patches.y.^qs.*patches.z.^rs;

```

Then evaluate the interpolation, setting faces to **inf** for error checking.

```

100 u=u0;
101 u([1:nEdge(1) end-nEdge(1)+1:end],:,:,:)=inf;
102 u(:,[1:nEdge(2) end-nEdge(2)+1:end],:,:)=inf;
103 u(:,:,1:nEdge(3) end-nEdge(3)+1:end,:)=inf;
104 ui=patchEdgeInt3(u(:));

```

All patches should have zero error: but need to either in **patchEdgeInt3** comment out **NaN** assignment of boundary values, or not test the two extreme patches here, or add code to omit NaNs here. High-order interpolation seems

to be more affected by round-off so relax error size.

```

114     error = ui-u0;
115     hist(log10(abs(error(abs(error)>1e-20))),-20:-6)
116     xlabel('log10 error'), pause(0.3)%??
117     maxError=max(abs(error(:)))
118     maxErrors=[maxErrors maxError];
119     assert(maxError<1e-10*4^ordCC ...
120         , 'failed divided difference interpolation')
121     disp('*** This divided difference test passed')

```

End the for-loops over various parameters.

```

128 end% for realisation
129 maxMaxErrorDividedDiffs = max(maxErrors)
130 disp('***** Passed all divided difference interpolation')
131 pause(1)

```

5.6.2.2 Test standard spectral interpolation

```

141 fprintf('\n\n***** Test standard spectral interpolation\n')
142 pause(1)

```

Test over various numbers of patches, random domain lengths and random ratios. Try realisations of random tests.

```
149 for realisation=1:nRealise
```

Choose and configure random sized domains, random sub-patch resolution, random size-ratios, random number of periodic-patches, randomly edge or mid-patch interpolation.

```

157 nEdge=randi(3,1,3)% =1,2, or 3
158 edgyInt = (rand>0.5)
159 Lx = 1+3*rand, Ly = 1+3*rand, Lz = 1+3*rand
160 xyzLim = [0 Lx 0 Ly 0 Lz]-[rand*[1 1] rand*[1 1] rand*[1 1]]
161 nSubP = nEdge.*((2-edgyInt)*randi(3,1,3)+1+edgyInt )
162 nPatch = randi([3 6],1,3)
163 dx = [Lx Ly Lz]./nPatch./nSubP.*rand(1,3)/2
164 configPatches3(@sin,xyzLim,'periodic',nPatches,0 ...
165     ,dx,nSubP,'EdgyInt',edgyInt,'nEdge',nEdge);

```

Choose a random number of fields, then generate trigonometric shape with random wavenumber and random phase shift. But if an even number of patches in either direction, then do not test the highest wavenumber because of aliasing problem.

```

175 nV=randi(3)
176 [nx,Nx]=size(squeeze(patches.x));
177 [ny,Ny]=size(squeeze(patches.y));
178 [nz,Nz]=size(squeeze(patches.z));
179 u0=nan(nx,ny,nz,nV,1,Nx,Ny,Nz);
180 for iV=1:nV

```

```

181     ks=floor( rand(1,3).*floor(([Nx Ny Nz]+1)/2) )
182     phis = pi*rand(1,3).*([2*ks~=[Nx Ny Nz])
183     % generate 8D array via auto-replication
184     u0(:,:,:,:,iV,1,:,:,:)=sin(2*pi*ks(1)*patches.x/Lx+phis(1)) ...
185             .*sin(2*pi*ks(2)*patches.y/Ly+phis(2)) ...
186             .*sin(2*pi*ks(3)*patches.z/Lz+phis(3));
187 end

```

Copy and nan the faces, then interpolate

```

193 u=u0;
194 u([1:nEdge(1) end-nEdge(1)+1:end],:,:,:)=nan;
195 u(:,[1:nEdge(2) end-nEdge(2)+1:end],:,:)=nan;
196 u(:,:,1:nEdge(3) end-nEdge(3)+1:end,:)=nan;
197 u=patchEdgeInt3(u(:));

```

Compute difference, ignoring the nans which should only be in the corners. If there is an error in the interpolation, then abort the script for checking: please record parameter values and inform us.

```

206 error = u-u0;
207 assert(all(~isnan(error(:))), 'found nans in the error!')
208 hist(log10(abs(error(abs(error)>1e-20))), -20:-6)
209 xlabel('log10 error'), pause(0.3)%??
210 normError=norm(error(:))
211 assert(normError<1e-10, '3D spectral interpolation failed')
212 disp('*** This spectral test passed')

```

End the for-loop over realisations

```

219 end
220 disp('***** All the spectral tests passed')
221 pause(1)

```

5.6.2.3 Check polynomial finite width interpolation

Check over various types and orders of interpolation, numbers of patches, random domain lengths and random ratios. (The `@sin` is a dummy.)

```

239 for realisations=1:nRealise
240     nEdge = randi(3,1,3)% =1,2, or 3
241     edgyInt = (rand>0.5)
242     nSubP = nEdge.*((2-edgyInt)*randi(2,1,3)+1+edgyInt )
243     ordCC = 2*randi(3)
244     nPatch = ordCC+randi(3,1,3)
245     xyzLim=5*[-rand(1,3); rand(1,3)]
246     dx = diff(xyzLim)./nPatch./nSubP.*rand(1,3)/2
247     configPatches3(@sin,xyzLim,'periodic',nPatch,ordCC ...
248                 ,dx,nSubP,'EdgyInt',edgyInt,'nEdge',nEdge);

```

Check multiple fields simultaneously Set profiles to be various powers of x, y, z , namely `ps`, `qs`, `rs`, and store as different ‘variables’ at each point.

```

258     [ps,qs,rs]=meshgrid(0:ordCC);
259     ps=reshape(ps,1,1,1,[]);
260     qs=reshape(qs,1,1,1,[]);
261     rs=reshape(rs,1,1,1,[]);
262     cs=2*rand(size(ps))-1;
263     u0=cs.*patches.x.^ps.*patches.y.^qs.*patches.z.^rs;

```

Then evaluate the interpolation.

```
269     ui=patchEdgeInt3(u0(:));
```

The interior patches should have zero error. Appear to need error tolerance of 10^{-8} because of the size of the domain and the high order of interpolation.

```

277     I=ordCC/2+1:nPatch(1)-ordCC/2;
278     J=ordCC/2+1:nPatch(2)-ordCC/2;
279     K=ordCC/2+1:nPatch(3)-ordCC/2;
280     error=ui(:,:,(:,:,I,J,K))-u0(:,:,(:,:,I,J,K));
281     assert(all(~isnan(error(:))), 'found nans in the error!')
282     hist(log10(abs(error(abs(error)>1e-20))), -20:-6)
283     xlabel('log10 error'), pause(0.3)%%
284     normError=norm(error(:))
285     assert(normError<5e-8 ...
286         , 'failed finite stencil polynomial interpolation')
287     disp('*** This finite stencil test passed')

```

End the for-loops over various parameters.

```
294 end%for realisation
295 disp('***** Passed all polynomial interpolation tests')
```

5.6.2.4 Finished

If no error messages, then all OK.

```
309 disp('***** All types of interpolation tests successful')
```

5.7 To do for patches

- Core averages code.
- Some staggered grid patches—although seems unnecessary.
- Adapt to maps in micro-time? Surely easy, just an example.
- Test hierarchy of patches.

6 Matlab parallel computation of the patch scheme

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For large-scale simulations, we here assume you have a compute cluster with many independent computer processors linked by a high-speed network. The functions we provide in our toolbox aim to distribute computations in parallel across the cluster. MATLAB’s *Parallel Computing Toolbox* empowers a reasonably straightforward way to implement this parallelisation.¹ The reason is that the patch scheme (Chapter 3) has a clear domain decomposition of assigning relatively few patches to each processor.

¹ This parallelisation is not written for, nor tested for, Octave.

The examples listed herein are all *Proof of Principle*: as coded they are all small enough that non-parallel execution is here much quicker than the parallel execution. One needs significantly larger and/or more detailed problems than these examples before parallel execution is effective.

As in all parallel cluster computing, interprocessor communication time all too often dominates. It is important to reduce communication as much as possible compared to computation. Consequently, parallel computing is only effective when there is a very large amount of microscale computation done on each processor per communication—all of the examples listed herein are quite small and so the parallel computation of these is much slower than serial computation. We guesstimate that the microscale code may need, per time-step, of the order of many millions of operations per processor in order for the parallelisation to be useful.

To help minimise communication in time-dependent problems we have drafted a special integrator `RK2mesoPatch`, [Section 6.4](#), that communicates between patches only on a meso-time ([Bunder et al. 2016](#)).

6.1 chanDispSpmd: simulation of a 1D shear dispersion via simulation on small patches across a channel

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6.1.3	microBurst function for Projective Integration	295
6.1.4	chanDispMicro(): heterogeneous 2D advection-diffusion in a long thin channel	296

Simulate 1D shear dispersion along long thin channel, dispersion that is emergent from micro-scale dynamics in 2D space. Use 1D patches as a Proof of Principle example of parallel computing with `spmd`. In this shear dispersion, although the micro-scale diffusivities are one-ish, the shear causes an effective longitudinal ‘diffusivity’ of the order of Pe^2 —which is typically much larger than the micro-scale diffusivity (Taylor 1953, e.g.).

The spatial domain is the channel (large) L -periodic in x and $|y| < 1$. Seek to predict a concentration field $c(x, y, t)$ satisfying the linear advection-diffusion PDE

$$\frac{\partial c}{\partial t} = -\text{Pe} u(y) \frac{\partial c}{\partial x} + \frac{\partial}{\partial x} \left[\kappa_x(y) \frac{\partial c}{\partial x} \right] + \frac{\partial}{\partial y} \left[\kappa_y(y) \frac{\partial c}{\partial y} \right]. \quad (6.1)$$

where Pe denotes a Peclet number, parabolic advection velocity $u(y) = \frac{3}{2}(1 - y^2)$ with noise, and parabolic diffusivity $\kappa_x(y) = \kappa_y(y) = (1 - y^2)$ with noise. The noise is to be multiplicative and log-normal to ensure advection and diffusion are all positive, and to be periodic in x .

For a microscale computation we discretise in space with x -spacing δx , and n_y points over $|y| < 1$ with spacing $\delta y := 2/n_y$ at $y_j := -1 + (j - \frac{1}{2})\delta y$, $j = 1 : n_y$. Our microscale discretisation of PDE (6.1) is then

$$\begin{aligned} \frac{\partial c_{ij}}{\partial t} &= -\text{Pe} u(y_j) \frac{c_{i+1,j} - c_{i-1,j}}{2\delta x} + \frac{d_{i,j+1/2} - d_{i,j-1/2}}{\delta y} + \frac{D_{i+1/2,j} - D_{i-1/2,j}}{\delta x}, \\ d_{ij} &:= \kappa_y(y_j) \frac{c_{i,j+1/2} - c_{i,j-1/2}}{\delta y}, \quad D_{ij} := \kappa_x(y_j) \frac{c_{i+1/2,j} - c_{i-1/2,j}}{\delta x}. \end{aligned} \quad (6.2)$$

These are coded in Section 6.1.4 for the computation.

Choose one of four cases:

- `theCase=1` is corresponding code without parallelisation (in this toy problem it is much the quickest because there is no expensive interprocessor communication);
- `theCase=2` illustrates that `RK2mesoPatch` invokes `spmd` computation if parallel has been configured.
- `theCase=3` shows how users explicitly invoke `spmd`-blocks around the time integration.

- `theCase=4` invokes projective integration for long-time simulation via short bursts of the micro-computation, bursts done within `spmd`-blocks for parallel computing.

First, clear all to remove any existing globals, old composites, etc—although a parallel pool persists. Then choose the case.

```
75  clear all
76  theCase = 1
```

The micro-scale PDE is evaluated at positions y_j across the channel, $|y| < 1$. The even indexed points are the collocation points for the PDE, whereas the odd indexed points are the half-grid points for specification of y -diffusivities.

```
86  ny = 7
87  y = linspace(-1,1,2*ny+1);
88  yj = y(2:2:end);
```

Set micro-scale advection (array 1) and diffusivity (array 2) with (roughly) parabolic shape ([Watt & Roberts 1995](#), [MacKenzie & Roberts 2003](#), e.g.). Here modify the parabola by a heterogeneous log-normal factor with specified period along the channel: modify the strength of the heterogeneity by the coefficient of `randn` from zero to perhaps one: coefficient 0.3 appears a good moderate value. Remember that `configPatches1` reshapes `cHetr` to 2D.

```
101 mPeriod = 4
102 cHetr = shiftdim([3/2 1],-1).*(1-y.^2) ...
103 .*exp(0.3*randn([mPeriod 2*ny+1 2]));
```

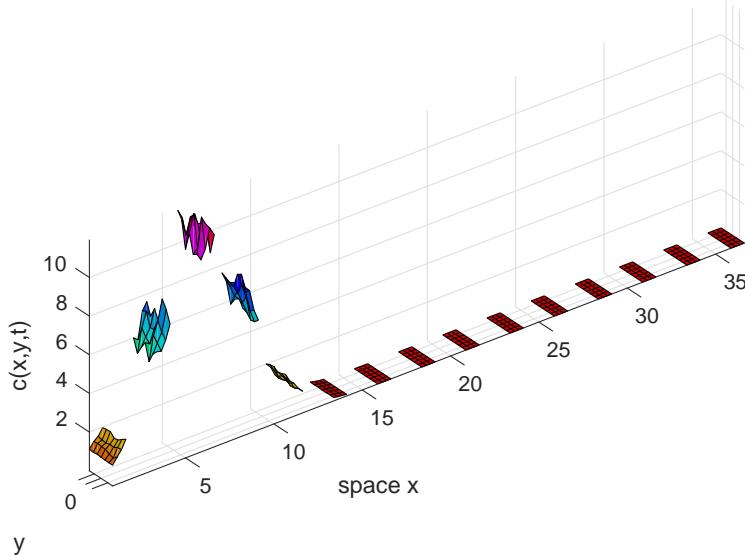
Configure the patch scheme with some arbitrary choices of domain, patches, size ratios. Choose some random order of interpolation to see the alternatives. Set `patches` information to be global so the info can be used for Cases 1–2 without being explicitly passed as arguments. Choose the parallel option if not Case 1, which invokes `spmd`-block internally, so that field variables become *distributed* across cpus.

```
118 if theCase<=2, global patches, end
119 nPatch=15
120 nSubP=2+mPeriod
121 ratio=0.2+0.2*(theCase<4)
122 Len=nPatch/ratio
123 ordCC=2*randi([0 3])
124 disp('**** Setting configPatches1')
125 patches = configPatches1(@chanDispMicro, [0 Len], nan ...
126 , nPatch, ordCC, ratio, nSubP, 'EdgyInt',true ...
127 , 'hetCoeffs',cHetr , 'parallel',(theCase>1) );
```

When using parallel then additional parameters to `patches` should be set within a `spmd` block (because `patches` is a co-distributed structure).

```
135 Peclet = 10
136 if theCase==1, patches.Pe = Peclet;
137 else      spmd, patches.Pe = Peclet; end
138 end
```

Figure 6.1: initial field $u(x, y, 0)$ of the patch scheme applied to a heterogeneous advection-diffusion PDE. Figure 6.2 plots the roughly smooth field values at time $t = 4$. In this example the patches are relatively large, ratio 0.4, for visibility.



6.1.1 Simulate heterogeneous advection-diffusion

Set initial conditions of a simulation as shown in Figure 6.1.

```
149 disp('**** Set initial condition and test dc0dt =')
150 if theCase==1
```

Without parallel processing, invoke the usual operations.

```
156 c0 = 10*exp(-(ratio*patches.x-2.5).^2/2) +0*yj;
157 c0 = c0.*(1+0.2*rand(size(c0)));
158 dc0dt = patchSys1(0,c0);
```

With parallel, we must use an `spmd`-block for computations: there is no difference in cases 2–4 here. Also, we must sometimes use `patches.codist` to explicitly code how to distribute new arrays over the cpus. Now `patchSys1` does not invoke `spmd` so higher level code must, as here. Even if `patches` is global, inside `spmd`-block we *must* pass it explicitly as a parameter to `patchSys1`.

```
171 else, spmd
172     c0 = 10*exp(-(ratio*patches.x-2.5).^2/2) +0*yj;
173     c0 = c0.*(1+0.2*rand(size(c0),patches.codist));
174     dc0dt = patchSys1(0,c0,patches)
175     end%spmd
176 end%if theCase
```

Integrate in time, either via the automatic `ode23` or via `RK2mesoPatch` which reduces communication between patches. By default, `RK2mesoPatch` does ten micro-steps for each specified meso-step in `ts`. For stability: with noise up

to 0.3, need micro-steps less than 0.005; with noise 1, need micro-steps less than 0.0015.

```
198 warning('Integrating system in time, wait patiently')
199 ts=4*linspace(0,1);
```

Go to the selected case.

```
205 switch theCase
```

1. For non-parallel, we could use `RK2mesoPatch` as indicated below, but instead choose to use standard `ode23` as here `patchSys1` accesses patch information via global `patches`. For post-processing, reshape each and every row of the computed solution to the correct array size—namely that of the initial condition.

```
217 case 1
218 % [cs,uerrs] = RK2mesoPatch(ts,c0);
219 [ts,cs] = ode23(@patchSys1,ts,c0(:));
220 cs=reshape(cs,[length(ts) size(c0)]);
```

2. In the second case, `RK2mesoPatch` detects a parallel patch code has been requested, but has only one cpu worker, so it auto-initiates an `spmd`-block for the integration. Both this and the next case return *composite* results, so just keep one version of the results.

```
232 case 2
233 cs = RK2mesoPatch(ts,c0);
234 cs = cs{1};
```

3. In this third case, a user could merge this explicit `spmd`-block with the previous one that sets the initial conditions.

```
243 case 3,spmd
244 cs = RK2mesoPatch(ts,c0,[],patches);
245 end%spmd
246 cs = cs{1};
```

4. In this fourth case, use Projective Integration (PI) over long times (`PIRK4` also works). Currently the PI is done serially, with parallel `spmd`-blocks only invoked inside function `aBurst()` ([Section 6.3.3](#)) to compute each burst of the micro-scale simulation. For a Peclet number of ten, the macro-scale time-step needs to be less than about 0.5 (which here is very little projection)—presumably the mean advection in a macro-step needs to be less than about the patch spacing. The function `microBurst()` here interfaces to `aBurst()` ([Section 6.1.3](#)) in order to provide shaped initial states, and to provide the patch information.

```
264 case 4
265 microBurst = @(tb0,xb0,bT) ...
266     aBurst(tb0 ,reshape(xb0,size(c0)) ,patches);
267 ts = 0:0.7:5
268 cs = PIRK2(microBurst,ts,gather(c0(:)));
269 cs = reshape(cs,[length(ts) size(c0)]);
```

End the four cases.

```
276 end%switch theCase
```

6.1.2 Plot the solution

Optionally set to save some plots to file.

```
287 if 0, global OurCf2eps, OurCf2eps=true, end
```

Animate the computed solution field over time

```
293 figure(1), clf, colormap(0.8* hsv)
```

First get the x -coordinates and omit the patch-edge values from the plot (because they are not here interpolated).

```
301 if theCase==1, x = patches.x;
302 else, spmd
303     x = gather( patches.x );
304 end%spmd
305     x = x{1};
306 end
307 x([1 end],:,:, :) = nan;
```

For every time step draw the concentration values as a set of surfaces on 2D patches, with a short pause to display animation.

```
315 nTimes = length(ts)
316 for l = 1:nTimes
```

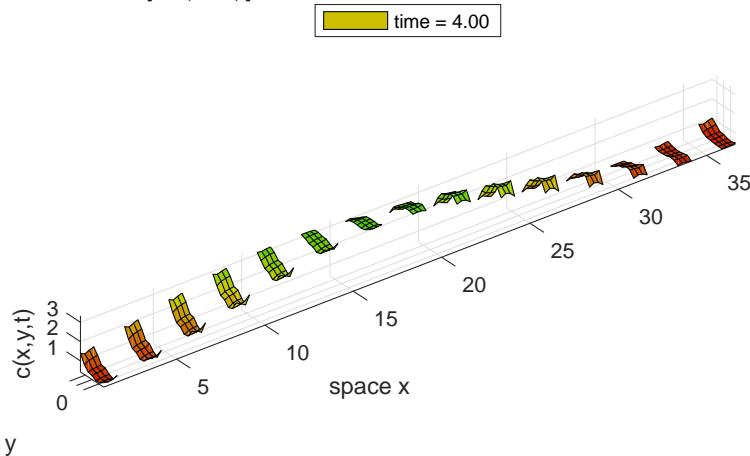
At each time, squeeze sub-patch data into a 3D array, permute to get all the x -variation in the first two dimensions, and reshape into x -variation for each and every (y).

```
325 c = reshape( permute( squeeze( ...
326     cs(l,:,:,:, :) ) , [1 3 2] ) ,numel(x) ,ny);
```

Draw surface of each patch, to show both micro-scale and macro-scale variation in space.

```
333 if l==1
334     hp = surf(x(:,yj,c'));
335     axis([0 Len -1 1 0 max(c(:))])
336     axis equal
337     xlabel('space $x$'), ylabel('$y$'); zlabel('$c(x,y,t)$')
338     ifOurCf2eps([mfilename 't0'])
339     legend(['time = ' num2str(ts(l),'%4.2f')] ...
340         , 'Location','north')
341     disp('**** pausing, press blank to animate')
342     pause
343 else
344     hp.ZData = c';
345     legend(['time = ' num2str(ts(l),'%4.2f')])
```

Figure 6.2: final field $c(x, y, 4)$ of the patch scheme applied to a heterogeneous advection-diffusion PDE (6.1) with heterogeneous factor log-normal, here distributed $\exp[\mathcal{N}(0, 1)]$.



```
346     pause(0.1)
347 end
```

Finish the animation loop, and optionally save the final plot to file, [Figure 6.2](#).

```
363 end%for over time
364 ifOurCf2eps([mfilename 'tFin'])
```

Macro-scale view Plot a macro-scale mesh of the predictions: at each of a selection of times, for every patch, plot the patch-mean value at the mean- x .

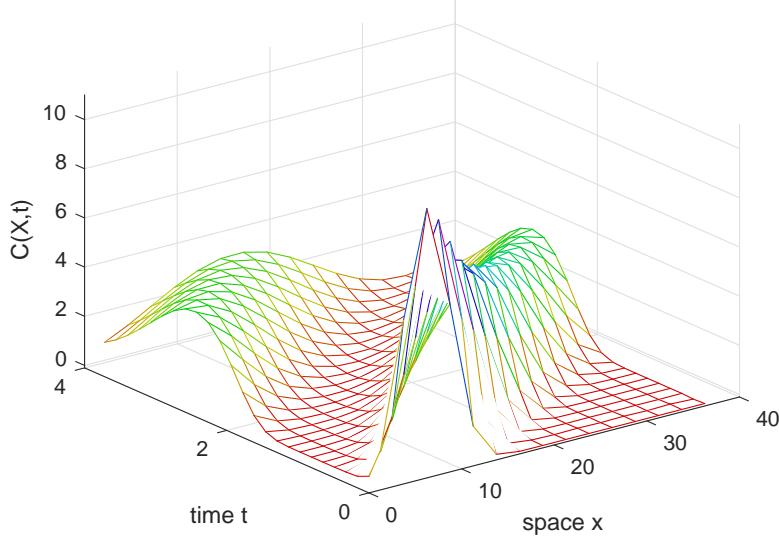
```
374 figure(2), clf, colormap(0.8*hsv)
375 X = squeeze(mean(x(2:end-1,:,:,:)));
376 C = squeeze(mean(mean(cs(:,2:end-1,:,:,:),2),3));
377 j = 1:ceil(nTimes/30):nTimes;
378 mesh(X,ts(j),C(j,:));
379 xlabel('space $x$'), ylabel('time $t$'), zlabel('$C(X, t)$')
380 zlim([-0.1 11])
381 ifOurCf2eps([mfilename 'Macro'])
```

6.1.3 microBurst function for Projective Integration

Projective Integration stability appears to require bursts longer than 0.2. Each burst is done in parallel processing. Here use `RK2mesoPatch` to take meso-steps, each with default ten micro-steps so the micro-scale step is 0.0033. With macro-step 0.5, these parameters usually give stable projective integration.

```
404 function [tbs,xbs] = aBurst(tb0,xb0,patches)
405     normx=max(abs(xb0(:)));
406     disp(['* aBurst t=' num2str(tb0) ' |x|=' num2str(normx)])
407     assert(normx<20,'solution exploding')
408     tbs = tb0+(0:0.033:0.2);
```

Figure 6.3: macro-scale view of heterogeneous advection-diffusion PDE along a (periodic) channel obtained via the patch scheme.



```

409     spmd
410         xb0 = codistributed(xb0,patches.codist);
411         xbs = RK2mesoPatch(tbs,xb0,[],patches);
412     end%spmd
413     xbs=reshape(xbs{1},length(tbs),[]);
414 end%function

```

Fin.

6.1.4 chanDispMicro(): heterogeneous 2D advection-diffusion in a long thin channel

This function codes the lattice heterogeneous diffusion inside the patches. For 4D input arrays of concentration c and spatial lattice x (via edge-value interpolation of `patchSys1`, Section 3.2), computes the time derivative (6.2) at each point in the interior of a patch, output in ct . The heterogeneous advects and diffusivities, $u_i(y_j)$ and $\kappa_i(y_{j+1/2})$, have previously been merged and stored in the one array `patches.cs` (2D).

```

22 function ct = chanDispMicro(t,c,p)
23     [nx,ny,~,~]=size(c); % micro-grid points in patches
24     ix = 2:nx-1;           % x interior points in a patch
25     dx = diff(p.x(2:3)); % x space step
26     dy = 2/ny;             % y space step
27     ct = nan+c;            % preallocate output array
28     pcs = reshape(p.cs,nx-1,[],2);

```

Compute the cross-channel flux using ‘ghost’ nodes at channel boundaries, so that the flux is zero at $y = \pm 1$ either because the boundary values are replicated so the differences are zero, or because the diffusivities in `cs` are zero at the channel boundaries.

```
38     ydif = pcs(ix,1:2:end,2) ...
39         .*(c(ix,[1:end end],:,:)-c(ix,[1 1:end],:,:))/dy;
```

Now evaluate advection-diffusion time derivative (6.2). Could use upwind advection and no longitudinal diffusion, or, as here, centred advection and diffusion.

```
48     ct(ix,:,:,:) = (ydif(:,2:end,:,:)-ydif(:,1:end-1,:,:))/dy ...
49         + diff(pcs(:,2:2:end,2).*diff(c))/dx^2 ...
50         - p.Pe*pcs(ix,2:2:end,1).*(c(ix+1,:,:,:)-c(ix-1,:,:,:))/(2*dx);
51 end% function
```

6.2 rotFilmSpmd: simulation of a 2D shallow water flow on a rotating heterogeneous substrate

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As an example application, consider the flow of a shallow layer of fluid on a solid flat rotating substrate, such as in spin coating (Wilson et al. 2000, Oron et al. 1997, §II.K, e.g.) or large-scale shallow water waves (Dellar & Salmon 2005, Hereman 2009, e.g.). Let $\vec{x} = (x, y)$ parametrise location on the rotating substrate, and let the fluid layer have thickness $h(\vec{x}, t)$ and move with depth-averaged horizontal velocity $\vec{v}(\vec{x}, t) = (u, v)$. We take as given (with its simplified physics) that the (non-dimensional) governing set of PDEs is the nonlinear system (Bunder & Roberts 2018, eq. (1), e.g.)

$$\frac{\partial h}{\partial t} = -\nabla \cdot (h\vec{v}), \quad (6.3a)$$

$$\frac{\partial \vec{v}}{\partial t} = \begin{bmatrix} -b & f \\ -f & -b \end{bmatrix} \vec{v} - (\vec{v} \cdot \nabla) \vec{v} - g \nabla h + \vec{\nabla} \cdot (\nu \vec{\nabla} \vec{v}), \quad (6.3b)$$

where $b(\vec{x})$ represents heterogeneous ‘bed’ drag, f is the Coriolis coefficient, g is the acceleration due to gravity, $\nu(\vec{x})$ is a heterogeneous ‘kinematic viscosity’, and we neglect surface tension.

The aim is to simulate the macroscale dynamics which (for constant b) is approximately that of the nonlinear diffusion $\partial h / \partial t \approx \frac{gb}{b^2+f^2} \vec{\nabla} \cdot (h \vec{\nabla} h)$ (Bunder & Roberts 2018, eq. (2)). But there is no known algebraic closure for the macroscale in the case of heterogeneous $b(\vec{x})$ and $\nu(\vec{x})$, nonetheless the patch scheme automatically predicts a sensible macroscale for such heterogeneous dynamics (Figure 6.5).

For the microscale computation, Section 6.2.4 discretises the PDEs (6.3) in space with x, y -spacing $\delta x, \delta y$.

Choose one of four cases:

- theCase=1 is corresponding code without parallelisation (in this toy problem it is much the quickest because there is no expensive communication);
- theCase=2 illustrates that RK2mesoPatch invokes spmd computation if parallel has been configured.
- theCase=3 shows how users explicitly invoke spmd-blocks around the time integration.

- `theCase=4` invokes projective integration for long-time simulation via short bursts of the micro-computation, bursts done within `spmd`-blocks for parallel computing.

First, clear all to remove any existing globals, old composites, etc—although a parallel pool persists. Then choose the case.

```
71  clear all
72  theCase = 1
```

Set micro-scale bed drag (array 1) and diffusivity (arrays 2–3) to be a heterogeneous log-normal factor with specified period: modify the strength of the heterogeneity by the coefficient of `randn` from zero to perhaps one: coefficient 0.3 appears a good moderate value.

```
82  mPeriod = 5
83  bnu = shiftdim([1 0.5 0.5], -1) ...
84      .*exp(0.3*randn([mPeriod mPeriod 3]));
```

Configure the patch scheme with these choices of domain, patches, size ratios—here each patch is square in space. In Cases 1–2, set `patches` information to be global so the info can be used without being explicitly passed as arguments.

```
96  if theCase<=2, global patches, end
```

In Case 4, double the size of the domain and use more separated patches accordingly, to maintain the spatial microscale grid spacing to be 0.055. Here use fourth order edge-based coupling between patches. Choose the parallel option if not Case 1, which invokes `spmd`-block internally, so that field variables become *distributed* across cpus.

```
108 nSubP = 2+mPeriod
109 nPatch = 9
110 ratio = 0.2+0.2*(theCase<4)
111 Len = 2*pi*(1+(theCase==4))
112 disp('**** Setting configPatches2')
113 patches = configPatches2(@rotFilmMicro, [0 Len], nan ...
114     , nPatch, 4, ratio, nSubP, 'EdgyInt',true ...
115     , 'hetCoeffs',bnu , 'parallel',(theCase>1) );
```

When using parallel, any additional parameters to `patches`, such as physical parameters for the microcode, must be set within a `spmd` block (because `patches` is a co-distributed structure). Here set frequency of substrate rotation, and strength of gravity.

```
125 f = 5, g = 1
126 if theCase==1, patches.f = f; patches.g = g;
127 else      spmd, patches.f = f; patches.g = g; end
128 end
```

6.2.1 Simulate heterogeneous advection-diffusion

Set initial conditions of a simulation as shown in [Figure 6.4](#). Here the initial condition is a (periodic) quasi-Gaussian in h and zero velocity \vec{v} , with additive

random perturbations.

```
141 disp('**** Set initial condition and test dhuv0dt =')
142 if theCase==1
```

When not parallel processing, invoke the usual operations. Here add a random noise to the velocity field, but keep $h(x, y, 0)$ smooth as shown by [Figure 6.4](#). The `shiftdim(...,-1)` moves the given row-vector of coefficients into the third dimension to become coefficients of the fields (h, u, v) , respectively.

```
153 huv0 = shiftdim([0.5 0 0],-1) ...
154     .*exp(-cos(patches.x)/2-cos(patches.y));
155 huv0 = huv0+0.1*shiftdim([0 1 1],-1).*rand(size(huv0));
156 dhuv0dt = patchSys2(0,huv0);
```

With parallel, we must use an `spmd`-block for computations: there is no difference in Cases 2–4 here. Also, we must sometimes explicitly tell functions how to distribute some initial condition arrays over the cpus. Now `patchSys2` does not invoke `spmd` so higher level code must, as here. Even if `patches` is global, inside an `spmd`-block we *must* pass `patches` explicitly as a parameter to `patchSys2`.

```
170 else, spmd
171     huv0 = shiftdim([0.5 0 0],-1) ...
172         .*exp(-cos(patches.x)/2-cos(patches.y));
173     huv0 = huv0+0.1*rand(size(huv0),patches.codist);
174     dhuv0dt = patchSys2(0,huv0,patches)
175     end%spmd
176 end%if theCase
```

Integrate in time, either via the automatic `ode23` or via `RK2mesoPatch` which reduces communication between patches. By default, `RK2mesoPatch` does ten micro-steps for each specified meso-step in `ts`. For stability: with noise up to 0.3, need micro-steps less than 0.0003; with noise 1, need micro-steps less than 0.0001.

```
201 warning('Integrating system in time, wait a minute')
202 ts=0:0.003:0.3;
```

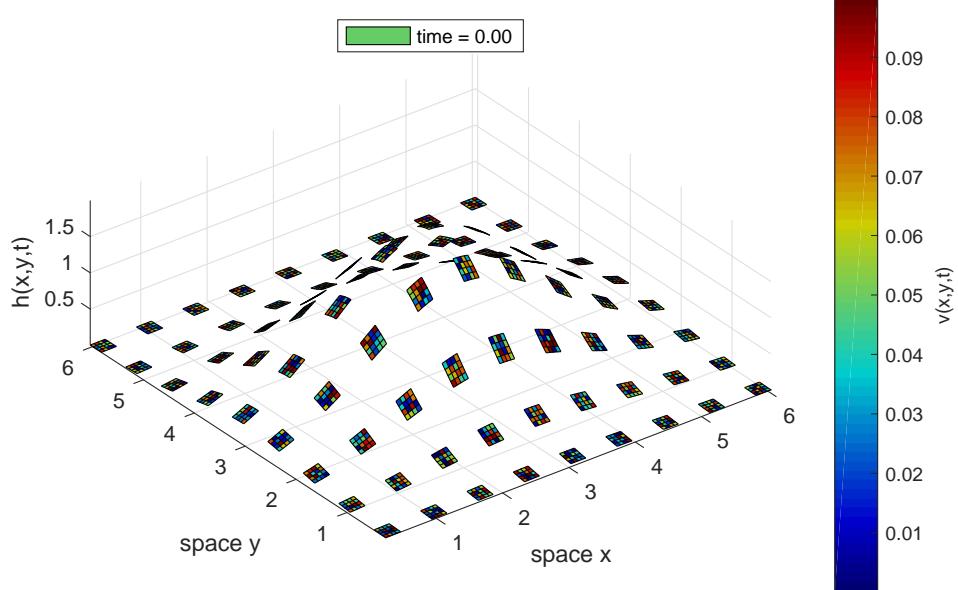
Go to the selected case.

```
208 switch theCase
```

1. For non-parallel, we could use `RK2mesoPatch` as indicated below, but instead choose to use standard `ode23` as here `patchSys2` accesses patch information via global `patches`. For post-processing, reshape each and every row of the computed solution to the correct array size—namely that of the initial condition.

```
220 case 1
221 %    tic,[huvs,uerrs] = RK2mesoPatch(ts,huv0);toc
222 [ts,huvs] = ode23(@patchSys2,[0 4],huv0(:));
223 huvs=reshape(huvs,[length(ts) size(huv0)]);
```

Figure 6.4: initial field $h(x, y, 0)$ of the patch scheme applied to the heterogeneous, shallow water, rotating substrate, PDE (6.3). The micro-scale sub-patch colour displays the initial y -direction velocity field $v(x, y, 0)$. Figure 6.5 plots the roughly smooth field values at time $t = 6$. In this example the patches are relatively large, ratio 0.4, for visibility.



2. In the second case, RK2mesoPatch detects a parallel patch code has been requested, but has only one cpu worker, so it auto-initiates an `spmd`-block for the integration. Both this and the next case return *composite* results, so just keep one version of the results.

```
235 case 2
236     huvs = RK2mesoPatch(ts,huv0);
237     huvs = huvs{1};
```

3. In this third case, a user could merge this explicit `spmd`-block with the previous one that sets the initial conditions.

```
246 case 3,spmd
247     huvs = RK2mesoPatch(ts,huv0,[],patches);
248 end%spmd
249 huvs = huvs{1};
```

4. In this fourth case, use Projective Integration (PI). Currently the PI is done serially, with parallel `spmd`-blocks only invoked inside function `aBurst()` (Section 6.2.3) to compute each burst of the micro-scale simulation. The macro-scale time-step needs to be less than about 0.1 (which here is not much projection). The function `microBurst()` interfaces to `aBurst()` (Section 6.2.3) in order to provide shaped initial states, and to provide the patch information.

```
264 case 4
265     microBurst = @(tb0,xb0,bT) ...
```

```

266      aBurst(tb0 ,reshape(xb0,size(huv0)) ,patches);
267      ts = 0:0.1:1
268      huvs = PIRK2(microBurst,ts,gather(huv0(:)));
269      huvs = reshape(huvs,[length(ts) size(huv0)]);
End the four cases.

276 end%switch theCase

```

6.2.2 Plot the solution

Optionally set to save some plots to file.

```
287 if 0, global OurCf2eps, OurCf2eps=true, end
```

Animate the computed solution field over time

```
293 figure(1), clf, colormap(0.8*jet)
```

First get the x -coordinates and omit the patch-edge values from the plot (because they are not here interpolated).

```

300 if theCase==1, x = patches.x;
301     y = patches.y;
302 else, spmd
303     x = gather( patches.x );
304     y = gather( patches.y );
305 end%spmd
306 x = x{1}; y = y{1};
307 end
308 x([1 end],:,:,(:,:,,:)) = nan;
309 y(:,:,1,[1 end],:,:, :) = nan;

```

Draw the field values as a patchy surface evolving over 100–200 time steps.

```
316 nTimes = length(ts)
317 for l = 1:ceil(nTimes/200):nTimes
```

At each time, squeeze sub-patch data fields into three 4D arrays, permute to get all the x/y -variations in the first/last two dimensions, and then reshape to 2D.

```

325 h = reshape( permute( squeeze( ...
326     huvs(l,:,:,:,1,1,:,:,:) ) ,[1 3 2 4]) ,numel(x),numel(y));
327 u = reshape( permute( squeeze( ...
328     huvs(l,:,:,:,2,1,:,:,:) ) ,[1 3 2 4]) ,numel(x),numel(y));
329 v = reshape( permute( squeeze( ...
330     huvs(l,:,:,:,3,1,:,:,:) ) ,[1 3 2 4]) ,numel(x),numel(y));

```

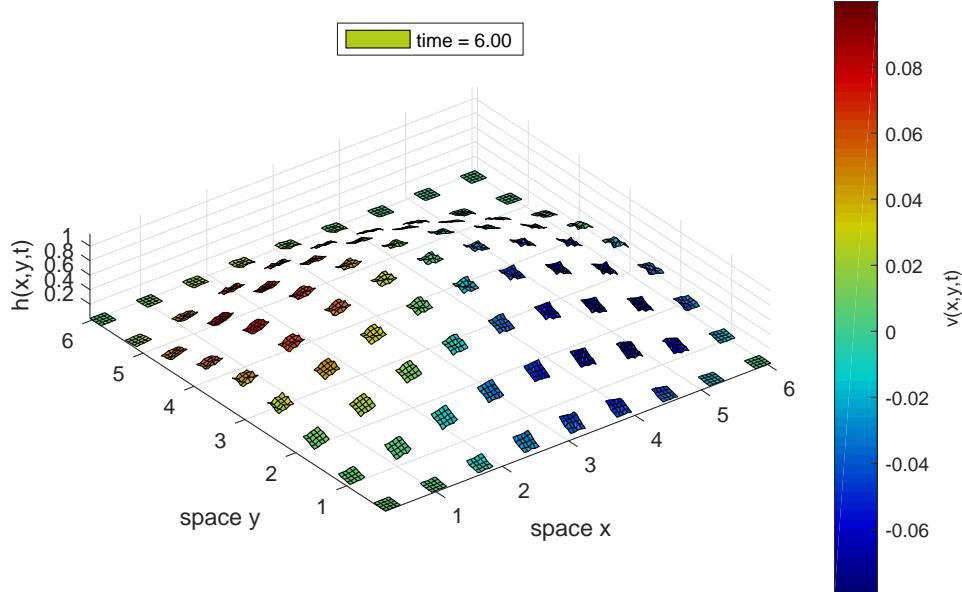
Draw surface of each patch, to show both micro-scale and macro-scale variation in space. Colour the surface according to the velocity v in the y -direction.

```

338 if l==1
339     hp = surf(x(:,y(:,h',v'));

```

Figure 6.5: final field $h(x, y, 6)$, coloured by $v(x, y, 6)$, of the patch scheme applied to the heterogeneous, shallow water, rotating substrate, PDE (6.3) with heterogeneous factors log-normal, here distributed $\exp[\mathcal{N}(0, 1)]$.



```

340     axis([0 Len 0 Len 0 max(h(:))])
341     c = colorbar; c.Label.String = 'v(x,y,t)';
342     legend(['time = ' num2str(ts(1),'%4.2f')] ...
343             , 'Location','north')
344     axis equal
345     xlabel('space $x$'), ylabel('space $y$'), zlabel('$h(x,y,t)$')
346     ifOurCf2eps([mfilename 't0'])
347     disp('**** pausing, press blank to begin animation')
348     pause
349 else
350     hp.ZData = h'; hp.CData = v';
351     legend(['time = ' num2str(ts(1),'%4.2f')])
352     pause(0.1)
353 end
370 end%for over time
371 ifOurCf2eps([mfilename 'tFin'])

```

Finish the animation loop, and optionally save the final plot to file, [Figure 6.5](#).

6.2.3 microBurst function for Projective Integration

Projective Integration stability appears to require bursts longer than 0.01. Each burst is done in parallel processing. Here use RK2mesoPatch to take meso-steps, each with default ten micro-steps so the micro-scale step is 0.0003. With macro-step 0.1, these parameters usually give stable projective integration.

```

388 function [tbs,xbs] = aBurst(tb0,xb0,patches)
389     normx=max(abs(xb0(:)));
390     disp(['* aBurst t=' num2str(tb0) ' |x|=' num2str(normx)])
391     assert(normx<20,'solution exploding')
392     tbs = tb0+(0:0.003:0.015);
393     spmd
394         xb0 = codistributed(xb0,patches.codist);
395         xbs = RK2mesoPatch(tbs,xb0,[],patches);
396     end%spmd
397     xbs=reshape(xbs{1},length(tbs),[]);
398 end%function

```

Fin.

6.2.4 rotFilmMicro(): 2D shallow water flow on a rotating heterogeneous substrate

This function codes the heterogeneous shallow water flow (6.3) inside 2D patches. The PDES are discretised on the multiscale lattice in terms of evolving variables h_{ijIJ} , u_{ijIJ} and v_{ijIJ} . For 6D input array `huv` (via edge-value interpolation of `patchEdgeInt2()`, Section 4.2), computes the time derivatives (6.3) at each point in the interior of a patch, output in `huvt`. The heterogeneous bed drag and diffusivities, b_{ij} and ν_{ij} , have previously been merged and stored in the array `patches.cs` (2D × 3): herein `patches` is named `p`.

```

24 function huvt = rotFilmMicro(t,huv,p)
25 [nx,ny,~]=size(huv); % micro-grid points in patches
26 i = 2:nx-1;           % x interior points in a patch
27 j = 2:ny-1;           % y interior points in a patch
28 dx = diff(p.x(2:3)); % x space step
29 dy = diff(p.y(2:3)); % y space step
30 huvt = nan+huv;      % preallocate output array

```

Set indices of fields in the arrays. Need to store different diffusivity values for the x, y -directions as they are evaluated at different points in space.

```

38 h=1; u=2; v=3;
39 b=1; nux=2; nuy=3;

```

Use a staggered micro-grid so that $h(i,j) = h_{ij}$, $u(i,j) = u_{i+1/2,j}$, and $v(i,j) = v_{i,j+1/2}$. We need the following to interpolate some quantities to other points on the staggered micro-grid. But the first two statements fill-in two needed corner values because they are not (currently) interpolated by `patchEdgeInt2()`.

```

51 huv(1,ny,u,:,:,:) = huv(2,ny,u,:,:,:)+huv(1,ny-1,u,:,:,:)
52             -huv(2,ny-1,u,:,:,:);
53 huv(nx,1,v,:,:,:) = huv(nx,2,v,:,:,:)+huv(nx-1,1,v,:,:,:)
54             -huv(nx-1,2,v,:,:,:);
55 v4u = (huv(i,j-1,v,:,:,:)+huv(i+1,j,v,:,:,:))
56             +huv(i,j,v,:,:,:)+huv(i+1,j-1,v,:,:,:))/4;

```

```

57 u4v = (huv(i,j+1,u,:,:,:)+huv(i-1,j,u,:,:,:))/4 ...
58     +huv(i,j,u,:,:,:)+huv(i-1,j+1,u,:,:,:))/4;
59 h2u = (huv(2:nx,:,h,:,:,:)+huv(1:nx-1,:,h,:,:,:))/2;
60 h2v = (huv(:,2:ny,h,:,:,:)+huv(:,1:ny-1,h,:,:,:))/2;

```

Evaluate conservation of mass PDE (6.3a) (needing averages of h at half-grid points):

```

67 huvt(i,j,h,:,:,:) = ...
68 - (h2u(i,j ,:,:,:,:).*huv(i ,j,u,:,:,:)) ...
69 - h2u(i-1,j ,:,:,:,:).*huv(i-1,j,u,:,:,:)/dx ...
70 - (h2v(i,j ,:,:,:,:).*huv(i,j ,v,:,:,:)) ...
71 - h2v(i,j-1,:,:,:,:).*huv(i,j-1,v,:,:,:))/dy ;

```

Evaluate the x -direction momentum PDE (6.3b) (needing to interpolate component v to u -points):

```

79 huvt(i,j,u,:,:,:) = ...
80 - p.cs(i,j,b).*huv(i,j,u,:,:,:)+ p.f.*v4u ...
81 - huv(i,j,u,:,:,:).*(huv(i+1,j,u,:,:,:)-huv(i-1,j,u,:,:,:))/(2*dx) ...
82 - v4u.* (huv(i,j+1,u,:,:,:)-huv(i,j-1,u,:,:,:))/(2*dy) ...
83 - p.g*(huv(i+1,j,h,:,:,:)-huv(i,j,h,:,:,:))/dx ...
84 + diff(p.cs(:,j,nux).*diff(huv(:,j,u,:,:,:),[],1),[],1)/dx^2 ...
85 + diff(p.cs(i,:,nuy).*diff(huv(i,:,u,:,:,:),[],2),[],2)/dy^2 ;

```

Evaluate the y -direction momentum PDE (6.3b) (needing to interpolate component u to v -points):

```

93 huvt(i,j,v,:,:,:) = ...
94 - p.cs(i,j,b).*huv(i,j,v,:,:,:)- p.f.*u4v ...
95 - u4v.* (huv(i+1,j,v,:,:,:)-huv(i-1,j,v,:,:,:))/(2*dx) ...
96 - huv(i,j,v,:,:,:).*(huv(i,j+1,v,:,:,:)-huv(i,j-1,v,:,:,:))/(2*dy) ...
97 - p.g*(huv(i,j+1,h,:,:,:)-huv(i,j,h,:,:,:))/dy ...
98 + diff(p.cs(:,j,nux).*diff(huv(:,j,v,:,:,:),[],1),[],1)/dx^2 ...
99 + diff(p.cs(i,:,nuy).*diff(huv(i,:,v,:,:,:),[],2),[],2)/dy^2 ;
100 end% function

```

6.3 homoDiff31spmd: computational homogenisation of a 1D dispersion via parallel simulation on small 3D patches of heterogeneous diffusion

Section contents

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Simulate effective dispersion along 1D space on 3D patches of heterogeneous diffusion as a Proof of Principle example of parallel computing with `spmd`. With only one patch in each of the y, z -directions, the solution simulated is strictly periodic in y, z with period `ratio`: there are only macro-scale variations in the x -direction. The discussion here only addresses issues with `spmd` parallel computing. For discussion on the 3D patch scheme with heterogeneous diffusion, see code and documentation for `homoDiffEdgy3` in [Section 5.4](#).

Choose one of four cases:

- `theCase=1` is corresponding code without parallelisation (in this toy problem it is much the quickest because there is no expensive communication);
- `theCase=2` for minimising coding by a user of `spmd`-blocks;
- `theCase=3` is for users happier to explicitly invoke `spmd`-blocks.
- `theCase=4` invokes projective integration for long-time simulation via short bursts of the micro-computation, bursts done within `spmd`-blocks for parallel computing.

First, clear all to remove any existing globals, old composites, etc—although a parallel pool persists. Then choose the case.

```
48 clear all
49 theCase = 1
```

Set micro-scale heterogeneity with various spatial periods in the three directions.

```
57 mPeriod = [4 3 2] %1+randperm(3)
58 cHetr = exp(0.3*randn([mPeriod 3]));
59 cHetr = cHetr*mean(1./cHetr(:))
```

Configure the patch scheme with some arbitrary choices of domain, patches, size ratios—here each patch is a unit cube in space. Choose some random order of interpolation. Set `patches` information to be global so the info can be used for Case 1 without being explicitly passed as arguments. Choose the parallel option if not Case 1, which invokes `spmd`-block internally, so that field variables become *distributed* across cpus.

```

73 if any(theCase==[1 2]), global patches, end
74 nSubP=mPeriod+2
75 nPatch=[9 1 1]
76 ratio=0.3
77 Len=nPatch(1)/ratio
78 ordCC=2*randi([0 3])
79 disp('**** Setting configPatches3')
80 patches = configPatches3(@heteroDiff3,[0 Len 0 1 0 1], nan ...
81 , nPatch, ordCC, [ratio 1 1], nSubP, 'EdgyInt',true ...
82 , 'hetCoeffs',cHetr , 'parallel',(theCase>1) );

```

6.3.1 Simulate heterogeneous diffusion

Set initial conditions of a simulation as shown in [Figure 6.6](#).

```

92 disp('**** Set initial condition and testing du0dt =')
93 if theCase==1

```

Without parallel processing, invoke the usual operations.

```

99 u0 = exp( -(patches.x-Len/2).^2/Len ...
100           -patches.y.^2/2-patches.z.^2 );
101 u0 = u0.* (1+0.2*rand(size(u0)));
102 du0dt = patchSys3(0,u0);

```

With parallel, must use an `spmd`-block for computations: there is no difference in cases 2–4 here. Also, we must sometimes explicitly code how to distribute some new arrays over the cpus. Now `patchSys3` does not invoke `spmd` so higher level code must, as here. Even if `patches` is global, inside `spmd`-block we must pass it explicitly as a parameter to `patchSys3`.

```

115 else, spmd
116     u0 = exp( -(patches.x-Len/2).^2/Len ...
117               -patches.y.^2/2-patches.z.^2/4 );
118     u0 = u0.* (1+0.2*rand(size(u0),patches.codist));
119     du0dt = patchSys3(0,u0,patches);
120     end%spmd
121 end%if theCase

```

Integrate in time. Use non-uniform time-steps for fun, and to show more of the initial rapid transients.

Alternatively, use `RK2mesoPatch` which reduces communication between patches, recalling that, by default, `RK2mesoPatch` does ten micro-steps for each specified step in `ts`. For unit cube patches, need micro-steps less than about 0.004 for stability.

```

144 warning('Integrating system in time, wait patiently')
145 ts=0.4*linspace(0,1,21).^2;

```

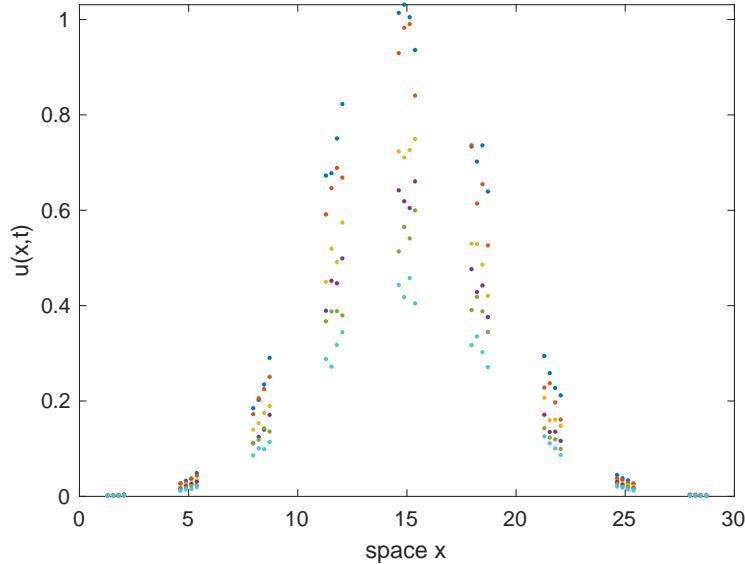
Go to the selected case.

```

151 switch theCase

```

Figure 6.6: initial field $u(x, y, z, 0)$ of the patch scheme applied to a heterogeneous diffusion PDE. The vertical spread indicates the extent of the structure in u in the cross-section variables y, z . Figure 6.7 plots the nearly smooth field values at time $t = 0.4$.



1. For non-parallel, we could use `RK2mesoPatch` as indicated below, but instead choose to use standard `ode23` as here `patchSys3` accesses patch information via global `patches`. For post-processing, reshape each and every row of the computed solution to the correct array size—that of the initial condition.

```

163 case 1
164 % [us,uerrs] = RK2mesoPatch(ts,u0);
165 [ts,us] = ode23(@patchSys3,ts,u0(:));
166 us=reshape(us,[length(ts) size(u0)]);

```

2. In the second case, `RK2mesoPatch` detects a parallel patch code has been requested, but has only one cpu worker, so it auto-initiates an `spmd`-block for the integration. Both this and the next case return *composite* results, so just keep one version of the results.

```

178 case 2
179 us = RK2mesoPatch(ts,u0);
180 us = us{1};

```

3. In this third case, a user could merge this explicit `spmd`-block with the previous one that sets the initial conditions.

```

189 case 3,spmd
190 us = RK2mesoPatch(ts,u0,[],patches);
191 end%spmd
192 us = us{1};

```

4. In this fourth case, use Projective Integration (PI) over long times (`PIRK4` also works). Currently the PI is done serially, with parallel

spmd-blocks only invoked inside function `aBurst()` ([Section 6.3.3](#)) to compute each burst of the micro-scale simulation. A macro-scale time-step of about 3 seems good to resolve the decay of the macro-scale ‘homogenised’ diffusion.² The function `microBurst()` here interfaces to `aBurst()` ([Section 6.3.3](#)) in order to provide shaped initial states, and to provide the patch information.

```

210 case 4
211     microBurst = @(tb0,xb0,bT) ...
212         aBurst(tb0 ,reshape(xb0,size(u0)) ,patches);
213     ts = 0:3:51
214     us = PIRK2(microBurst,ts,gather(u0(:)));
215     us = reshape(us,[length(ts) size(u0)]);
222 end%switch theCase

```

End the four cases.

6.3.2 Plot the solution

Optionally save some plots to file.

```
233 if 0, global OurCf2eps, OurCf2eps=true, end
```

Animate the solution field over time. Since the spatial domain is long in x and thin in y, z , just plot field values as a function of x .

```

241 figure(1), clf
242 if theCase==1
243     x = reshape( patches.x(2:end-1,:,:,:) ,[],1);
244 else, spmd
245     x = reshape(gather( patches.x(2:end-1,:,:,:) ),[],1);
246 end%spmd
247 x = x{1};
248 end

```

For every time step draw the field values as dots and pause for a short display.

```
255 nTimes = length(ts)
256 for l = 1:length(ts)
```

At each time, squeeze interior point data into a 4D array, permute to get all the x -variation in the first two dimensions, and reshape into x -variation for each and every (y, z) .

```
265 u = reshape( permute( squeeze( ...
266     us(1,2:end-1,2:end-1,2:end-1,:) ) ,[1 4 2 3]) ,numel(x),[]);
```

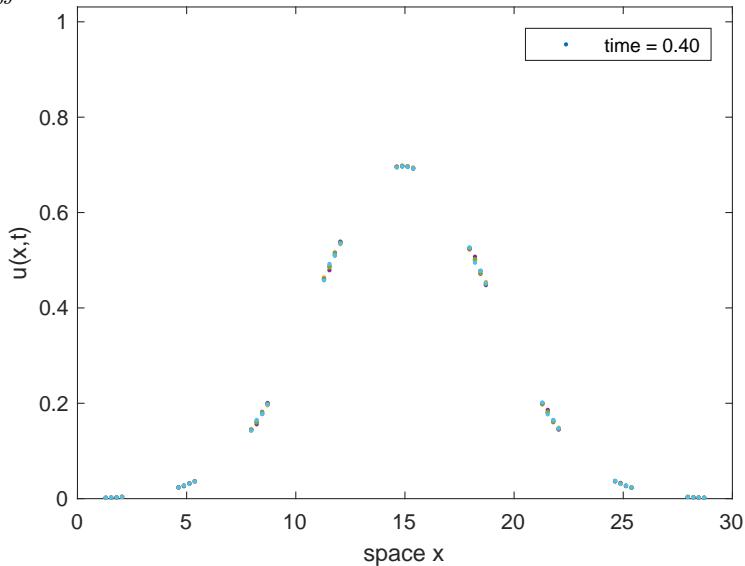
Draw point data to show spread at each cross-section, as well as macro-scale variation in the long space direction.

```
273 if l==1
274     hp = plot(x,u,'.');

```

² Curiously, `PIG()` appears to suffer unrecoverable instabilities with its variable step size!

Figure 6.7: final field $u(x, y, z, 0.4)$ of the patch scheme applied to a heterogeneous diffusion PDE.



```

275 axis([0 Len 0 max(u(:))])
276 xlabel('space $x$'), ylabel('$u(x,y,z,t)$')
277 ifOurCf2eps([mfilename 't0'])
278 legend(['time = ' num2str(ts(1),'%4.2f')])
279 disp('**** pausing, press blank to animate')
280 pause
281 else
282 for p=1:size(u,2), hp(p).YData=u(:,p); end
283 legend(['time = ' num2str(ts(1),'%4.2f')])
284 pause(0.1)
285 end

```

Finish the animation loop, and optionally output the final plot, Figure 6.7.

```

298 end%for over time
299 ifOurCf2eps([mfilename 'tFin'])

```

6.3.3 microBurst function for Projective Integration

Projective Integration stability seems to need bursts longer than 0.2. Here take ten meso-steps, each with default ten micro-steps so the micro-scale step is 0.002. With macro-step 3, these parameters usually give stable projective integration (but not always).

```

315 function [tbs,xbs] = aBurst(tb0,xb0,patches)
316     normx=max(abs(xb0(:)));
317     disp(['aBurst t = ' num2str(tb0) ' |x| = ' num2str(normx)])
318     assert(normx<10,'solution exploding')
319     tbs = tb0+(0:0.02:0.2);
320     spmd
321         xb0 = codistributed(xb0,patches.codist);

```

```
322      xbs = RK2mesoPatch(tbs,xb0,[],patches);  
323      end%spmd  
324      xbs=reshape(xbs{1},length(tbs),[]);  
325  end%function
```

Fin.

6.4 RK2mesoPatch()

This is a Runge–Kutta, 2nd order, integration of a given deterministic system of ODEs on patches. It invokes meso-time updates of the patch-edge values in order to reduce interpolation costs, and uses a linear variation in edge-values over the meso-time-step (Bunder et al. 2016, case $Q = 2$). This function is aimed primarily for large problems executed on a computer cluster to markedly reduce expensive communication between computers.

If using within projective integration, it appears quite tricky to get all the time-steps chosen appropriately. One has to choose times for: the micro-scale time-step, the meso-time interval between communications, the longer meso-time burst length, and the macro-scale integration time-step.

```
27 function [xs,errs] = RK2mesoPatch(ts,x0,nMicro,patches)
28 if nargin<4, global patches, end
```

Input

- `patches.fun()` is a function such as `dxdt=fun(t,x,patches)` that computes the right-hand side of the ODE $d\vec{x}/dt = \vec{f}(t, \vec{x})$ where \vec{x} is a vector/array, t is a scalar, and the result \vec{f} is a correspondingly sized vector/array.
- `x0` is an vector/array of initial values at the time `ts(1)`.
- `ts` is a vector of meso-scale times to compute the approximate solution, say in \mathbb{R}^ℓ for $\ell \geq 2$.
- `nMicro`, optional, default 10, is the number of micro-time-steps taken for each meso-scale time-step.
- `patches` struct set by `configPatchesn` and provided as either as parameter, or as a global variable.

Output

- `xs`, 5/7/9D (depending upon `nD`) array of length $\ell \times \dots$ of approximate solution vector/array at the specified times. But, if using parallel computing via `spmd`, then `xs` is a *composite* 5/7/9D array, so outside of an `spmd`-block access a single copy of the array via `xs{1}`. Similarly for `errs`.
- `errs`, column vector in \mathbb{R}^ℓ of local error estimate for the step from t_{k-1} to t_k .

Code of RK2 integration Set default number of micro-scale time-steps in each requested meso-scale step of `ts`. Cannot use `nargin` inside explicit `spmd`, but can use it if the `spmd` is already active from the code that invokes this function.

```
79 if nargin<3|isempty(nMicro), nMicro=10; end
```

If patches are set to be in parallel (there must be a parallel pool), but only one worker available (i.e., not already inside `spmd`), then invoke function recursively inside `spmd`. Q: is `numlabs` defined without the parallel computing toolbox??

```

89 if isequal(class(patches), 'Composite') && numlabs==1
90     spmd,
91         [xs,errs] = RK2mesoPatch(ts,x0,nMicro,patches);
92     end% spmd
93     assert(isequal(class(xs) , 'Composite'), ' xs  not composite')
94     assert(isequal(class(errs),'Composite'), 'errs not composite')
95     return
96 end

```

Set the number of space dimensions from the number stored patch-size ratios.

```
104 nD = length(patches.ratio);
```

Set the micro-time-steps and create storage for outputs.

```

110 dt = diff(ts)/nMicro;
111 xs = nan([numel(ts) size(x0)]);
112 errs = nan(numel(ts),1);

```

Initialise first result to the given initial condition, and evaluate the initial time derivative into `f1`. Use inter-patch interpolation to ensure edge values of the initial condition are defined and are reasonable.³

```

127 switch nD
128     case 1, x0 = patchEdgeInt1(x0,patches);
129         xs(1,:,:,:,:) = gather(x0);
130     case 2, x0 = patchEdgeInt2(x0,patches);
131         xs(1,:,:,:,:, :) = gather(x0);
132     case 3, x0 = patchEdgeInt3(x0,patches);
133         xs(1,:,:,:,:, :, :) = gather(x0);
134     end;%switch nD
135 errs(1) = 0;
136 f1 = patches.fun(ts(1),x0,patches);

```

Compute the meso-time-steps from t_k to t_{k+1} , copying the derivative `f1` at the end of the last micro-time-step to be the derivative at the start of this one.

```
145 for k = 1:numel(dt)
```

Perform meso-time burst with the new interpolation for edge values, and an interpolation of the time derivatives to get derivative estimates of the edge-values.

³ These `gather()` functions cause all-to-all interprocessor communication once every meso-step. Maybe better to use distributed array instead, (although need to then need to put time index last instead of first??), but we need to do some inter-cpu communication in order to estimate errors.

```

153     switch nD
154         case 1, dx0 = patchEdgeInt1(f1,patches);
155         case 2, dx0 = patchEdgeInt2(f1,patches);
156         case 3, dx0 = patchEdgeInt3(f1,patches);
157     end;%switch nD

```

Perform the micro-time steps.

```

163     for m=1:nMicro
164         f0 = f1;
165         % assert(iscodistributed(f0),'f0 not codist')

```

For all micro-time derivative evaluations, include that the edge values are varying according to the estimate made at the start of the meso-time-step.

```

173     switch nD
174         case 1, f0([1 end],:,:,:,:)=dx0([1 end],:,:,:,:);
175         case 2, f0([1 end],:,:, :, :, :)=dx0([1 end],:,:, :, :, :);
176             f0(:,[1 end],:,:, :, :, :)=dx0(:,[1 end],:,:, :, :, :);
177         case 3
178             f0([1 end],:,:, :, :, :, :, :)=dx0([1 end],:,:, :, :, :, :, :);
179             f0(:,[1 end],:,:, :, :, :, :, :)=dx0(:,[1 end],:,:, :, :, :, :, :);
180             f0(:,:, [1 end],:,:, :, :, :, :, :)=dx0(:,:, [1 end],:,:, :, :, :, :, :);
181     end;%switch nD
182     % assert(iscodistributed(f0),'f0 not codist two')

```

Simple second-order accurate Runge–Kutta micro-scale time-step.

```

189     xh = x0+f0*dt(k)/2;
190     % assert(iscodistributed(xh),'xh not codist')
191     fh = patches.fun(ts(k)+dt(k)*(m-0.5),xh,patches);
192     % assert(iscodistributed(fh),'fh not codist one')
193     switch nD
194         case 1, fh([1 end],:,:,:,:)=dx0([1 end],:,:,:,:);
195         case 2, fh([1 end],:,:, :, :, :)=dx0([1 end],:,:, :, :, :);
196             fh(:,[1 end],:,:, :, :, :)=dx0(:,[1 end],:,:, :, :, :);
197         case 3
198             fh([1 end],:,:, :, :, :, :, :)=dx0([1 end],:,:, :, :, :, :, :);
199             fh(:,[1 end],:,:, :, :, :, :, :)=dx0(:,[1 end],:,:, :, :, :, :, :);
200             fh(:,:, [1 end],:,:, :, :, :, :, :)=dx0(:,:, [1 end],:,:, :, :, :, :, :);
201     end;%switch nD
202     % assert(iscodistributed(fh),'fh not codist two')
203     x0 = x0+fh*dt(k);
204     % assert(iscodistributed(x0),'x0 not codist two')

```

End the burst of micro-time-steps.

```

210     end

```

At the end of each meso-step burst, refresh the interpolate of the edge values, evaluate time-derivative, and temporarily fill-in edges of derivatives (to ensure error estimate is reasonable).

```

219     switch nD
220         case 1, x0 = patchEdgeInt1(x0,patches);
221             xs(k+1,:,:,:,:) = gather(x0);
222         case 2, x0 = patchEdgeInt2(x0,patches);
223             xs(k+1,:,:,:,:,::) = gather(x0);
224         case 3, x0 = patchEdgeInt3(x0,patches);
225             xs(k+1,:,:,:,:,::,:,:) = gather(x0);
226     end;%switch nD
227 % assert(iscodistributed(x0),'x0 not codist three')
228 f1 = patches.fun(ts(k+1),x0,patches);
229 switch nD
230     case 1, f1([1 end],:,:,:,:)=dx0([1 end],:,:,:,:);
231     case 2, f1([1 end],:,:,:,:,::)=dx0([1 end],:,:,:,:,::);
232         f1(:,[1 end],:,:,:,:)=dx0(:,[1 end],:,:,:,:,:);
233     case 3
234         f1([1 end],:,:,:,:,:,:)=dx0([1 end],:,:,:,:,:,:,:);
235         f1(:,[1 end],:,:,:,:,:,:)=dx0(:,[1 end],:,:,:,:,:,:);
236         f1(:,:,1,[1 end],:,:,:,:)=dx0(:,:,1,[1 end],:,:,:,:);
237 end;%switch nD

```

Use the time derivative at t_{k+1} to estimate an error by storing the difference with what Simpson's rule would estimate over the last micro-time step performed.

```

245     f0=f0-2*fh+f1;
246 % assert(iscodistributed(f0),'f2ndDeriv not codist')
247     errs(k+1) = sqrt(gather(mean(f0(:).^2,'omitnan')))*dt(k)/6;
248 end%for-loop
249 end%function

```

End of the function with results returned in `xs` and `errs`.

6.5 To do

- Detailed profiling of the spmd communication to seek better parallelisation.

Appendix A Create, document and test algorithms

- Upon ‘finalising’ a version of the toolbox:
 1. pdflatex and bibtex `Doc/eqnFreeDevMan.tex` to ensure all is documented properly;
 2. execute `bibexport eqnFreeDevMan` to update the local bibliographic data-file;
 3. pdflatex `Doc/eqnFreeUserMan.tex`, several times, to get a shorter and more user friendly version;
 4. replace the root file `eqnFreeUserMan-newest.pdf` by a renamed copy of the new `Doc/eqnFreeUserMan.pdf`
- To create and document the various functions, we adapt an idea due to Neil D. Lawrence of the University of Sheffield in order to interleave MATLAB/Octave code, and its documentation in LaTeX ([Table A.2](#)).
- Each class of toolbox functions is located in separate folders in the repository, say `Dir`.
- Create a LaTeX file `Dir/funs.tex`: establish as one LaTeX chapter that `\input{../Dir/*.m}`s the files of the functions in the class, example scripts of use, and possibly test scripts, [Table A.1](#).
- Each such `Dir/funs.tex` file is to be included from the main LaTeX file `Doc/docBody.tex` so that people can most easily work on one chapter at a time:
 - create a ‘link’ file `Doc/funs.tex` whose only active content is the command `\input{../Dir/funs.tex}`;
 - put `\include{funs}` into `Doc/docBody.tex`;
 - in `Doc/docBody.tex` modify the `\graphicspath` command to include `{../Dir/Figs}`.
- Each toolbox function is documented as a separate section, within its chapter, with tests and examples as separate sections.
- Each function-section and test-section is to be created as a MATLAB/Octave `Dir/*.m` file, say `Dir/fun1.m`, so that users simply invoke the function in MATLAB/Octave as usual by `fun1(...)`.

Some editors may need to be told that `fun1.m` is a LaTeX file. For example, TexShop on the Mac requires one to execute (once) in a Terminal

```
defaults write TeXShop OtherTeXExtensions -array-add "m"
```

- [Table A.2](#) gives the template for the `Dir/*.m` function-sections. The format for a example/test-section is similar.

- Any figures from examples should be generated and then saved for later inclusion with the following (which finally works properly for MATLAB 2017+)

```
set(gcf, 'PaperUnits', 'centimeters', 'PaperPosition', [0 0 14 10]);% cm
print('-depsc2', 'filename')
```

If it is a suitable replacement for an existing graphic, then move it into the `Dir/Figs` folder. Include such a graphic into the LaTeX document with (do *not* postfix with `.eps` or `.pdf`)

```
\includegraphics[scale=0.9]{filename}
```

- In figures and other graphics, do *not* resize/scale fixed width constructs: instead use `\linewidth` to configure large-scale layout, `em` for small-widths, and `ex` for small-heights.
- For every function, generally include at the start of the function a simple example of its use. The example is only to be executed when the function is invoked with no input arguments (`if nargin==0`).

When appropriate, if a function is invoked with no output arguments (`if nargout==0`), then draw some reasonable graph of the results.

- In all MATLAB/Octave code, prefer camel case for variable names (not underscores).
- When a function is ‘finalised’, wrap (most) of the lines to be no more than 60 characters so that readers looking at the source can read the plain text reasonably.
- In the documentation (e.g., [Higham 1998](#), Ch. 4): write actively, not passively (e.g., avoid “-tion” words, and avoid “is/are verbed” phrases); avoid wishy-washy “can”; use the present tense; cross-reference precisely; avoid useless padding such as “note that”; and so on.

Table A.1: example `Dir/*.tex` file to typeset in the master document a function-section, say `fun.m`, and maybe the test/example-sections.

```

1 % input *.m files for ... Author, date
2 %!TEX root = ../Doc/eqnFreeDevMan.tex
3 \chapter{...}
4 \label{ch:...}
5 \localtableofcontents
6 Introduction...
7 \input{../Dir/fun.m} % prefix associated files with 'fun'
8 \input{../Dir/funExample.m}
9 ...
10 \begin{devMan}
11 \section{To do}
12 ...
13 \section{Miscellaneous tests}
14 \input{../Dir/funTest.m}
15 ...
16 \end{devMan}
```

Table A.2: template for a function-section `Dir/*.m` file.

```

1 % Short explanation for users typing "help fun"
2 % Author, date
3 %!TEX root = ../Doc/eqnFreeDevMan.tex
4 %{
5 \section{\texttt{...}: ...}
6 \label{sec:...}
7 \localtableofcontents
8 \subsection{Introduction}
9 Overview LaTeX explanation.
10 \begin{matlab}
11 %}
12 function ...
13 %{
14 \end{matlab}
15 \paragraph{Input} ...
16 \paragraph{Output} ...
17 \begin{devMan}
18 Repeated as desired:
19 LaTeX between end-matlab and begin-matlab
20 \begin{matlab}
21 %}
22 Matlab code between \%} and \%{
23 %{
24 \end{matlab}
25 Concluding LaTeX before following final lines.
26 \end{devMan}
27 %}
```

Appendix B Aspects of developing a ‘toolbox’ for patch dynamics

Chapter contents

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This appendix documents sketchy further thoughts on aspects of the development.

B.1 Macroscale grid

The patches are to be distributed on a macroscale grid: the j th patch ‘centred’ at position $\vec{X}_j \in \mathbb{X}$. In principle the patches could move, but let’s keep them fixed in the first version. The simplest macroscale grid will be rectangular (`meshgrid`), but we plan to allow a deformed grid to secondly cater for boundary fitting to quite general domain shapes \mathbb{X} . And plan to later allow for more general interconnect networks for more topologies in application.

B.2 Macroscale field variables

The researcher/user has to know an appropriate set of macroscale field variables $\vec{U}(t) \in \mathbb{R}^{d_U}$ for each patch. For example, first they might be a simple average over a core of a patch of all of the micro-field variables; second, they might be a subset of the average micro-field variables; and third in general the macro-variables might be a nonlinear function of the micro-field variables (such as temperature is the average speed squared). The core might be just one point, or a sizeable fraction of the patch.

The mapping from microscale variable to macroscale variables is often termed the restriction.

In practice, users may not choose an appropriate set of macro-variables, so will eventually need to code some diagnostic to indicate a failure of the assumed closure.

B.3 Boundary and coupling conditions

The physical domain boundary conditions are distinct from the conditions coupling the patches together. Start with physical boundary conditions of periodicity in the macroscale.

Second, assume the physical boundary conditions are that the macro-variables are known at macroscale grid points around the boundary. Then the issue is to adjust the interpolation to cater for the boundary presence and shape. The coupling conditions for the patches should cater for the range of Robin-like boundary conditions, from Dirichlet to Neumann. Two possibilities arise: direct imposition of the coupling action ([Roberts & Kevrekidis 2007](#)), or control by the action.

Third, assume that some of the patches have some edges coincident with the boundary of the macroscale domain \mathbb{X} , and it is on these edges that macroscale physical boundary conditions are applied. Then the interpolation from the core of these edge patches is the same as the second case of prescribed boundary macro-variables. An issue is that each boundary patch should be big enough to cater for any spatial boundary layers transitioning from the applied boundary condition to the interior slow evolution.

Alternatively, we might have the physical boundary condition constrain the interpolation between patches.

Often microscale simulations are easiest to write when ‘periodic’ in microscale space. To cater for this we should also allow a control at perhaps the quartiles of a micro-periodic simulator.

B.4 Mesotime communication

Since communication limits large scale parallelism, a first step in reducing communication will be to implement only updating the coupling conditions when necessary. Error analysis indicates that updating on times longer the microscale times and shorter than the macroscale times can be effective (Bunder et al. 2016). Implementations can communicate one or more derivatives in time, as well as macroscale variables.

At this stage we can effectively parallelise over patches: first by simply using Matlab’s `parfor`. Probably not using a GPU as we probably want to leave GPUs for the black-box to utilise within each patch.

B.5 Projective integration

Have coded several schemes.

Should not need an implicit scheme as the fast dynamics are meant to be only in the micro variables, and the slow dynamics only in the macroscale variables. However, it could be that the macroscale variables have fast oscillations and it is only the amplitude of the oscillations that are slow. Perhaps need to detect and then fix or advise, perhaps via DMD.

A further stage is to implement a projective integration scheme for stochastic macroscale variables: this is important because the averaging over a core of microscale roughness will almost invariably have at least some stochastic legacy effect. [Calderon \(2007\)](#) did some useful research on stochastic projective integration.

B.6 Lift to many internal modes

In most problems the number of macroscale variables at any given position in space, $d_{\vec{U}}$, is less than the number of microscale variables at a position, $d_{\vec{u}}$; often much less ([Kevrekidis & Samaey 2009](#), e.g.). In this case, every time we start a patch simulation we need to provide $d_{\vec{u}} - d_{\vec{U}}$ data at each position in the patch: this is lifting. The first methodology is to first guess, then run repeated short bursts with reinitialisation, until the simulation reaches a slow manifold (e.g., `cdmc()`). Then run the real simulation.

If the time taken to reach a local quasi-equilibrium is too long, then it is likely that the macroscale closure is bad and the macroscale variables need to be extended.

A second step is to cater for cases where the slow manifold is stochastic or is surrounded by fast waves: when it is hard to detect the slow manifold, or the slow manifold is not attractive.

B.7 Macroscale closure

In some circumstances a researcher/user will not code in a restriction the appropriately set of macroscale variables for a complete closure of the macroscale. For example, in thin film fluid dynamics at low Reynolds number the only macroscale variable is the fluid depth; however, at higher Reynolds number, circa ten, the inertia of the fluid becomes important and the macroscale variables must additionally include a measure of the mean lateral velocity/momentum ([Roberts & Li 2006](#), e.g.).

At some stage we need to detect any flaw in the closure implied by a restriction, and perhaps suggest additional appropriate macroscale variables, or at least their characteristics. Indeed, a poor closure and a stochastic slow manifold are really two faces of the same problem: the problem is that the chosen macroscale variables do not have a unique evolution in terms of themselves. A good resolution of the issue will account for both faces.

B.8 Exascale fault tolerance

MATLAB/Octave is probably not an appropriate vehicle to deal with real exascale faults. However, we should cater by coding procedures for fault tolerance and testing them at least synthetically. Eventually provide hooks to a user routine to be invoked under various potential scenarios. The nature of fault tolerant algorithms will vary depending upon the scenario, even assuming that each patch burst is executed on one CPU (or closely coupled CPUS): if there are many more CPUS than patches, then maybe simply duplicate all patch simulations; if many fewer CPUS than patches, then an asynchronous scheduling of patch bursts should effectively cater for recomputation of failed bursts; if comparable CPUS to patches, then more subtle action is needed.

Once mesotime communication and projective integration is provided, a recomputation approach to intermittent hardware faults should be effective because we then have the tools to restart a burst from available macroscale data. Should also explore proceeding with a lower order interpolation that misses the faulty burst—because an isolated lower order interpolation probably will not affect the global order of error (it does not in approximating some boundary conditions ([Gustafsson 1975, Svard & Nordstrom 2006](#))).

B.9 Link to established packages

Several molecular/particle/agent based codes are well developed and used by a wide community of researchers. Plan to develop hooks to use some such codes as the microscale simulators on patches. First, may connect to LAMMPS ([Plimpton et al. 2016](#)). Second, will evaluate performance, issues, and then consider what other established packages are most promising.

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