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`

Contents

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/uoa1184615/EquationFreeGit. Place the folders `Patch` and `ProjInt` of this toolbox in a path searched by Matlab/Octave (but *not* the folder `SandpitPlay` as that contains experimental development functions). 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 analytically 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 given 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 (2016*b*) established high-order consistency for the 1D staggered patch scheme, and Divahar et al. (2022), Bunder et al. (2021) established excellent 2D staggered patch schemes for waves.
- A heterogeneous microscale is more difficult, but Bunder et al. (2020), Bunder & Roberts (2022) developed a new 'edgy' inter-patch interpolation that is analytically proven to be excellent for simulating the macroscale homogenised dynamics of microscale heterogeneous systems in multiple space dimensions—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 powerful and flexible Matlab/Octave toolbox of equation-free algorithms. Initially the algorithms are basic, and the ongoing program is developing 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 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

Chapter contents

2.1 Introduction

This section provides some good projective integration functions (Gear & Kevrekidis 2003*b*,*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. (2005*a*), 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.

Schematic for Projective Integration scheme

Set microsolver
Code a function that interfaces to your 'black-box' microsolver, including the burst time, `bT`, of the microsolver. Possible aids:

- Use the Patch functions (Figure 3.1) to simulate a large-scale PDE, lattice, etc.
- Use `cmdc()` as a wrapper for the microsolver if the slow variables may change significantly over the microsolver burst.

Set macro simulator
Set the vector of output times `tSpan/Tspan`, and set initial values `x0`.

- If using `PIRKn()`, then intervals between times are the projective time-steps.
- If using `PIG()`, then intervals between times are as needed by `macroInt`.

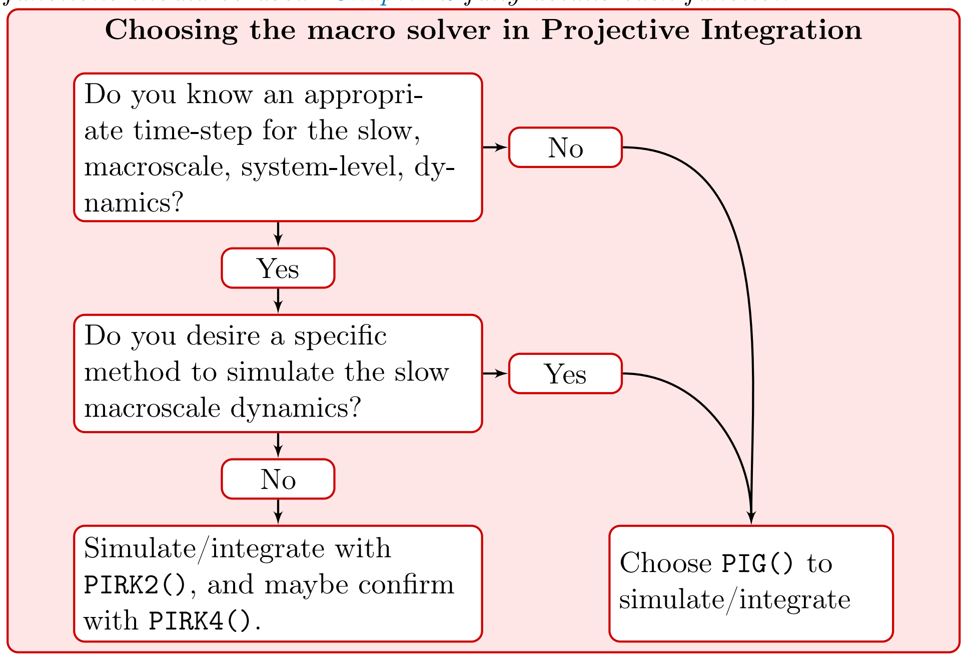
Do Projective Integration
Invoke the appropriate Projective Integration function as, e.g., `x = PIRK2(microBurst, tSpan, x0)`, or `[t,x] = PIG(macroInt, microBurst, Tspan, x0)`. Additional optional outputs inform you of the microscale.

Set lifting/ restriction If needed, set functions `restrict()` and `lift()` to convert between macro and micro problems/ variables. These are optional arguments to the Projective Integration functions.

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

Section contents

2.2.1 Introduction

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

```
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`.

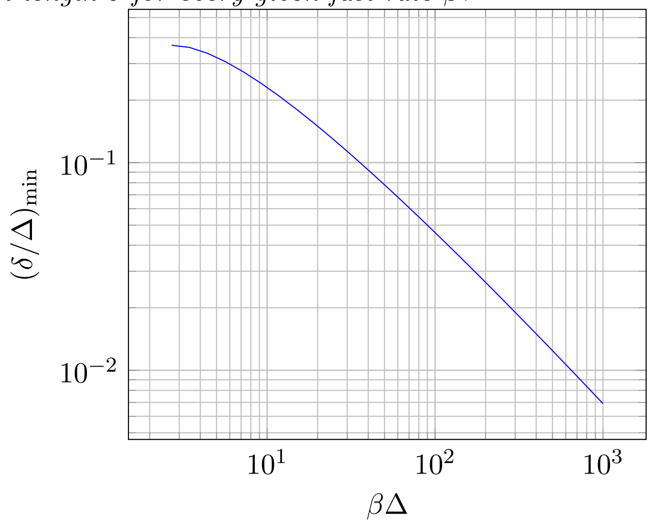
  – Outputs: `tOut`, the column vector of solution times; and `xOut`, an array in which each *row* contains the system state at corresponding times.

  Be wary that for very large scale separations (such as `MMepsilon<1e-5` in the Michaelis–Menten 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.

```
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, $\Delta =$ `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

```
if nargin==0
```

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

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

(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 $0 \le t \le 6$ 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 $\Delta = 1$.

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

Upon finishing execution of the example, exit this function.

```
return
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 $x =$ x(1) and $y =$ 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.

```
function [ts, xs] = MMburst(ti, xi, bT)
    global MMepsilon
    dMMdt = @(t,x) [ -x(1)+(x(1)+0.5)*x(2)
        1/MMepsilon*( x(1)-(x(1)+1)*x(2) ) ];
    if ~exist('OCTAVE_VERSION','builtin')
    [ts, xs] = ode23(dMMdt, [ti ti+bT], xi);
    else % octave version
    [ts, xs] = odeOct(dMMdt, [ti ti+bT], xi);
    end
end
```

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

2.2.3 The projective integration code

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

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

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

```
nArgOut=nargout();
saveMicro = (nArgOut>1);
saveFullMicro = (nArgOut>3);
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.

```
x0 = reshape(x0,1,[]);
[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.

```
tSpan(1) = relax_t(end);
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.

```
if saveMicro
    tms = cell(nT,1);
    xms = cell(nT,1);
    tms{1} = reshape(relax_t,[],1);
    xms{1} = relax_x0;
    if saveFullMicro
        rm.t = cell(nT,1);
        rm.x = cell(nT,1);
        if saveSvf
            svf.t = nan(2*nT-2,1);
            svf.dx = nan(2*nT-2,length(x0));
        end
    end
end
```

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

```
roundingTol = 1e-8;
for jT = 2:nT
    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.

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

Run the first application of the microBurst; 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.

```
        [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.

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

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

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

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

```
Dt = tSpan(jT)-t1(end);
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).

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

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

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

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

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

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

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

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

```
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.

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

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

```
        if saveFullMicro
            rm.t{jT} = [reshape(t2,[],1); nan];
            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.

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

End the main loop over all the macro-steps.

```
end
```

Overwrite `x(1,:)` with the specified initial condition `tSpan(1)`.

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

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

```
if saveMicro
    tms = cell2mat(tms);
    xms = cell2mat(xms);
    if saveFullMicro
        rm.t = cell2mat(rm.t);
        rm.x = cell2mat(rm.x);
    end
end
```

2.2.4 If no output specified, then plot the simulation

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

This concludes `PIRK2()`.

```
end
```

2.3 `egPIMM`: Example projective integration of Michaelis–Menton kinetics

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

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

(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.

```
clear all, close all
global MMepsilon
MMepsilon = 0.1
```

First, the end of this section encodes the computation of bursts of the Michaelis–Menten 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–Menten system, at time $t = 0$, of $(x, y) = (1, 0)$ (off the slow manifold).

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

Figure 2.4 plots the macroscale results showing the long time decay of the Michaelis–Menten 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.

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

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

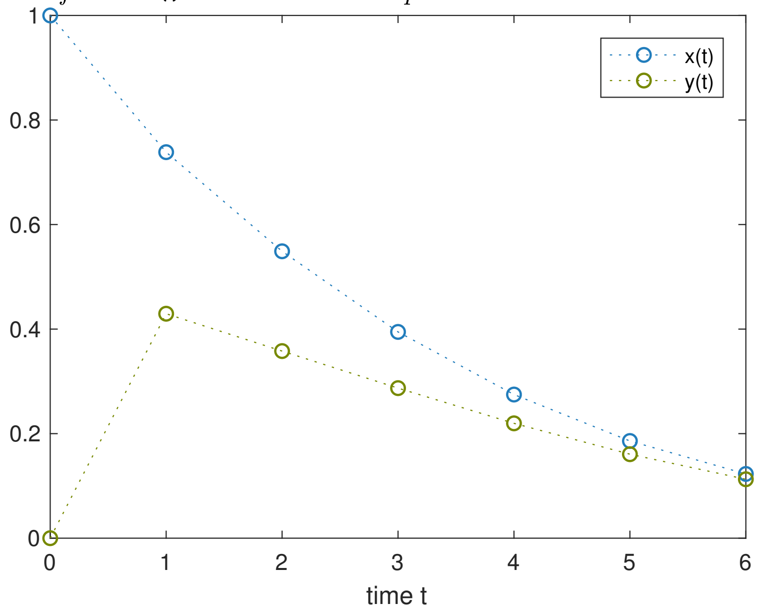


Figure 2.5 plots the macroscale and microscale results—also showing that the initial burst is by default twice as long. Observe the slow variable $x(t)$ is also affected by the initial transient (hence other schemes which 'freeze' slow variables are less accurate).

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 2003*a*, 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.

```
ts = 0:-1:-5
[xs,tMicro,xMicro] = PIRK2(@MMburst, ts, 0.2*[1;1], 3*MMepsilon);
figure, plot(ts,xs,'o:',tMicro,xMicro)
xlabel('time t'), legend('x(t)','y(t)')
title('backward integration showing points with bursts')
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 $x =$ `x(1)` and $y =$ `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.

```
function [ts, xs] = MMburst(ti, xi, bT)
    global MMepsilon
    dMMdt = @(t,x) [ -x(1)+(x(1)+0.5)*x(2)
        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.

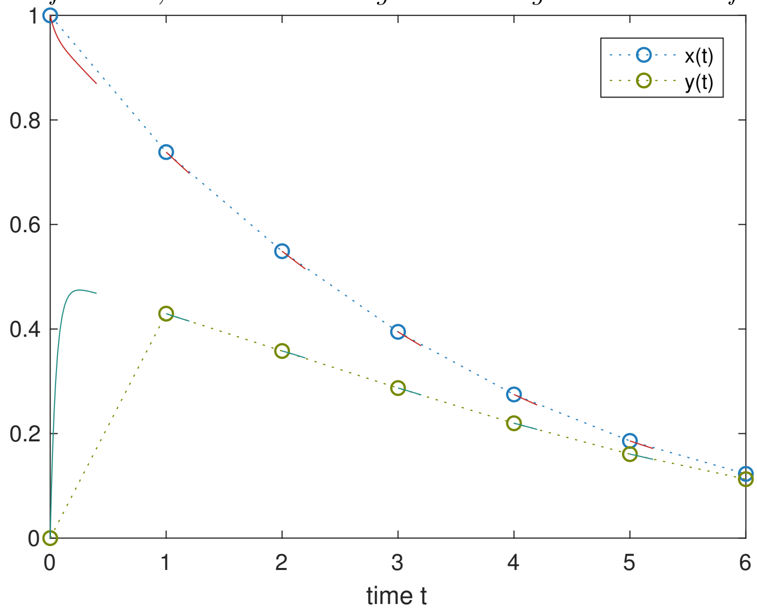
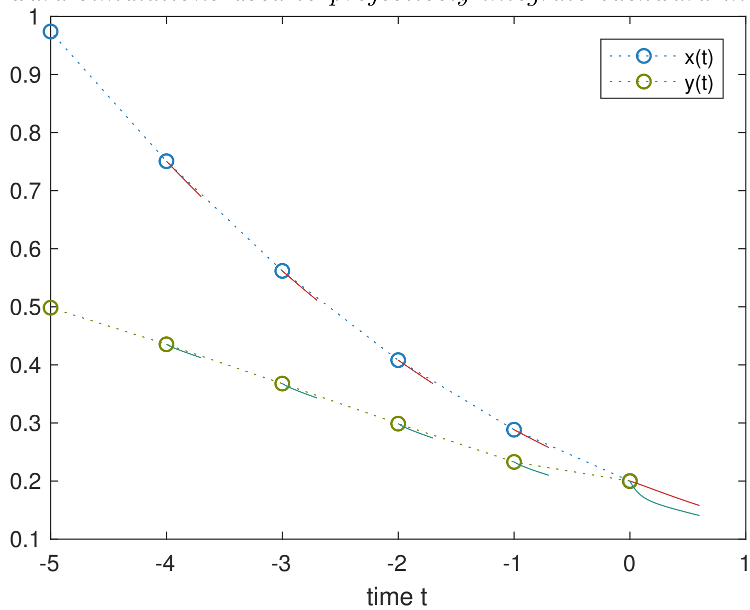


Figure 2.6: Michaelis–Menten enzyme kinetics at $\epsilon = 0.1$ simulated backward with the projective integration of `PIRK2()`: the microscale bursts show the short forward simulations used to projectively integrate backward in time.



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

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

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

Section contents

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. (2005*b*), uses a backward projection so that the simulation time is unchanged after running the microscale simulator.

```
function [T,X,tms,xms,svf] = PIG(macroInt,microBurst,Tspan,x0 ...
                                    ,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] = 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 ith *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.

- `X`, an $L \times N$ array of the computed solution: the ith *row* of `X`, `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(...)`

- `tms`, optional, is an ℓ-dimensional column vector containing microscale times with bursts, each burst separated by `NaN`;
- `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

- `svf`, optional, a struct containing the Projective Integration estimates of the slow vector field.
  - `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()`.
  - `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

```
if nargin==0
```

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

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

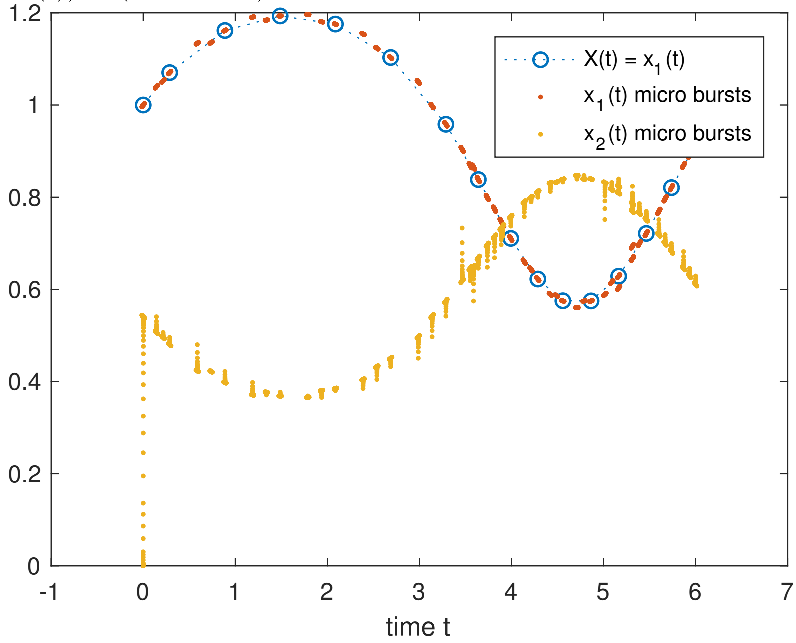
The macroscale variable is $X(t) = x_1(t)$, and the evolution dX/dt is unclear. With initial condition $X(0) = 1$, the following code computes and plots a solution of the system (2.1) over time $0 \le t \le 6$ for parameter $\epsilon = 10^{-3}$(Figure 2.7). Whenever needed by `microBurst()`, the microscale 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.

```
epsilon = 1e-3;
dxdt=@(t,x) [ cos(x(1))*sin(x(2))*cos(t)
              ( 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 $\Delta \le 1$ 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* $(x_1(t), x_2(t)) =$ *(red, yellow) dots.*




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

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

```
restrict = @(x) x(1);
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 $0 \le t \le 6$ 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 2003*a*, Frewen et al. 2009).

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

Plot output of this projective integration.

```
figure, plot(Ts,Xs,'o:',tms,xms,'.')
title('Projective integration of singularly perturbed ODE')
xlabel('time t')
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.

```
return
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.

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

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

```
nArgOut = nargout();
saveMicro = (nArgOut>2);
saveSvf = (nArgOut>4);
```

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

```
nT = length(Tspan)-1;
nx = length(x0);
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.

```
if nargin<7
    microBurst = @(t,x) cdmc(microBurst,t,x);
else
warning(['A ' class(cdmcFlag) ' seventh input to PIG().'...
 ' PIG will not use constraint-defined manifold computing.'])
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.

```
[relaxT,x0MicroRelax] = microBurst(Tspan(1),x0);
xMicroLast = x0MicroRelax(end,:).';
X0Relax = restrict(xMicroLast);
```

Update the initial time.

```
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.

```
if saveMicro
    tms=cell(nT+1,1); xms=cell(nT+1,1);
    n=1;
    tms{n} = reshape(relaxT,[],1);
    xms{n} = x0MicroRelax;

    if saveSvf
        svf.T = cell(nT+1,1);
        svf.dX = cell(nT+1,1);
    else
        svf = [];
    end
else
    tms = []; xms = []; svf = [];
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

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

Run a microBurst from the given macroscale initial values.

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

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

```
  X2 = restrict(xMicroTmp(end,:));
  X1 = restrict(xMicroTmp(end-1,:));
  dt = tTmp(end)-tTmp(end-1);
  dXdt = (X2 - X1).'/dt;
```

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

```
  if saveMicro
      n=n+1;
      tms{n} = [reshape(tTmp,[],1); nan];
      xms{n} = [xMicroTmp; nan(1,nx)];
      if saveSvf
          svf.T{n-1} = t;
          svf.dX{n-1} = dXdt;
      end
```

```
  end
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.

```
PIF = @(t,x) PIFun(t,x);
[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.

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

Concatenate all the additional requested outputs into arrays.

```
if saveMicro
    tms = cell2mat(tms);
    xms = cell2mat(xms);
    if saveSvf
        svf.T = cell2mat(svf.T);
        svf.dX = cell2mat(svf.dX);
    end
end
```

2.4.4 If no output specified, then plot the simulation

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

This concludes `PIG()`.

```
end
```

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

Section contents

2.5.1 Introduction

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

```
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

```
if nargin==0
```

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

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

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 $\Delta = -1$.

```
global MMepsilon
MMepsilon = 0.1
ts = 0:-1:-5
bT = MMepsilon*log(abs(ts(2)-ts(1))/MMepsilon)
[x,tms,xms,rm,svf] = PIRK4(@MMburst, ts, 0.2*[1;1], bT);
figure, plot(ts,x,'o:',tms,xms)
xlabel('time t'), legend('x(t)','y(t)')
title('Backwards-time projective integration of Michaelis--Menten')
```

Upon finishing execution of the example, exit this function.

```
return
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 $x =$ `x(1)` and $y =$ `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.

```
function [ts, xs] = MMburst(ti, xi, bT)
    global MMepsilon
    dMMdt = @(t,x) [ -x(1)+(x(1)+0.5)*x(2)
        1/MMepsilon*( x(1)-(x(1)+1)*x(2) ) ];
    if ~exist('OCTAVE_VERSION','builtin')
    [ts, xs] = ode23(dMMdt, [ti ti+bT], xi);
    else % octave version
    [ts, xs] = odeOct(dMMdt, [ti ti+bT], xi);
    end
end
```

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

```
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.

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

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

```
nArgOut = nargout();
saveMicro = (nArgOut>1);
saveFullMicro = (nArgOut>3);
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.

```
x0 = reshape(x0,1,[]);
[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.

```
tSpan(1) = relax_t(end);
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.

```
if saveMicro
    tms = cell(nT,1);
    xms = cell(nT,1);
    tms{1} = reshape(relax_t,[],1);
    xms{1} = relax_x0;
    if saveFullMicro
        rm.t = cell(nT,1);
        rm.x = cell(nT,1);
        if saveSvf
            svf.t = nan(4*nT-4,1);
            svf.dx = nan(4*nT-4,length(x0));
        end
    end
end
```

Loop over the macroscale time-steps

```
for jT = 2:nT
    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.

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

```
        t2=nan; xm2=nan(1,size(xm1,2));
        t3=nan; t4=nan; xm3=xm2; xm4 = xm2; dx1=xm2; dx2=xm2;
    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.

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

Check for round-off error.

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

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

```
    Dt = tSpan(jT)-t1(end);
    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()`).

```
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.

```
    xint = xm1(end,:) + (Dt/2-abT)*dx1;
    [t2,xm2] = microBurst(T+Dt/2, xint, bT);
    del = t2(end)-t2(end-1);
    dx2 = (xm2(end,:)-xm2(end-1,:))/del;

    xint = xm1(end,:) + (Dt/2-abT)*dx2;
    [t3,xm3] = microBurst(T+Dt/2, xint, bT);
    del = t3(end)-t3(end-1);
    dx3 = (xm3(end,:)-xm3(end-1,:))/del;

    xint = xm1(end,:) + (Dt-abT)*dx3;
    [t4,xm4] = microBurst(T+Dt, xint, bT);
    del = t4(end)-t4(end-1);
    dx4 = (xm4(end,:)-xm4(end-1,:))/del;
```

Check for round-off error.

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

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

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

```
    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.

```
    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 `NaN`s.

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

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

```
        if saveFullMicro
            rm.t{jT} = [reshape(t2,[],1); nan;...
                        reshape(t3,[],1); nan;...
                        reshape(t4,[],1); nan];
            rm.x{jT} = [xm2; nan(1,size(xm2,2));...
                        xm3; nan(1,size(xm2,2));...
                        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.

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

End of the main loop of all macro-steps.

```
end
```

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

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

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

```
if saveMicro
    tms = cell2mat(tms);
    xms = cell2mat(xms);
    if saveFullMicro
```

```
        rm.t = cell2mat(rm.t);
        rm.x = cell2mat(rm.x);
    end
end
```

2.5.3 If no output specified, then plot the simulation

```
if nArgOut==0
    figure, plot(tSpan,x,'o:')
    title('Projective Simulation with PIRK4')
end
```

This concludes `PIRK4()`.

```
end
```

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.

```
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.

```
[t1,x1] = feval(microBurst,t0,x0);
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`.

```
dxdt = (x1(end,:) - x1(end-1,:))/(t1(end) - t1(end-1));
x0 = x1(end,:)-2*bT*dxdt;
t0 = t1(1)-bT;
[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)`.

```
ts = [t1(:); t2(:)];
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.

```
clear
rand('seed',1) % albeit discouraged in Matlab
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,

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

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

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

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

```
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.

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

We implement the PI scheme, saving the coarse states in `x`, the 'trusted' applications of the microsolver in `tms` and `xms`, and the additional applications of the microsolver in `rm` (the second, third and fourth outputs are optional).

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

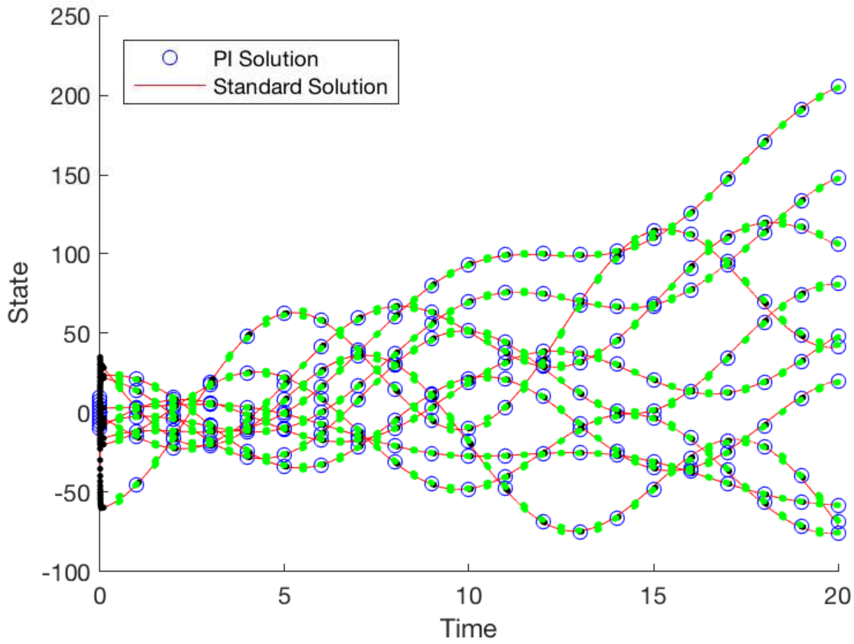
To verify, we also compute the trajectories using a standard integrator.

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

Figure 2.8 plots the output.

```
clf()
hold on
PI_sol=plot(tSpan,x,'bo');
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.*




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

Save plot to a file.

```
if ~exist('OCTAVE_VERSION','builtin')
set(gcf,'PaperUnits','centimeters','PaperPosition',[0 0 14 10])
print('-depsc2','PIRKexample')
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 $\texttt{dt} \leq 1/|\texttt{fastband}(1)|$ and the time to simulate with each application of the microsolver, `bT`, should be larger than or equal to $1/|\texttt{fastband}(2)|$. 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

```
function [ts, xs] = linearBurst(ti, xi, varargin)
global dxdt
dt = 0.001;
ts = ti+(0:dt:0.05)';
nts = length(ts);
xs = NaN(nts,length(xi));
```

```
xs(1,:)=xi;
for k=2:nts
    xi = xi + dt*dxdt(ts(k),xi.').';
    xs(k,:)=xi;
end
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`.

```
clear all, close all
```

Set time scale separation and the underlying ODEs:

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

```
epsilon = 1e-4;
dxdt=@(t,x) [ cos(x(1))*sin(x(2))*cos(t)
              (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.

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

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

```
x0 = [1 0.9];
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).

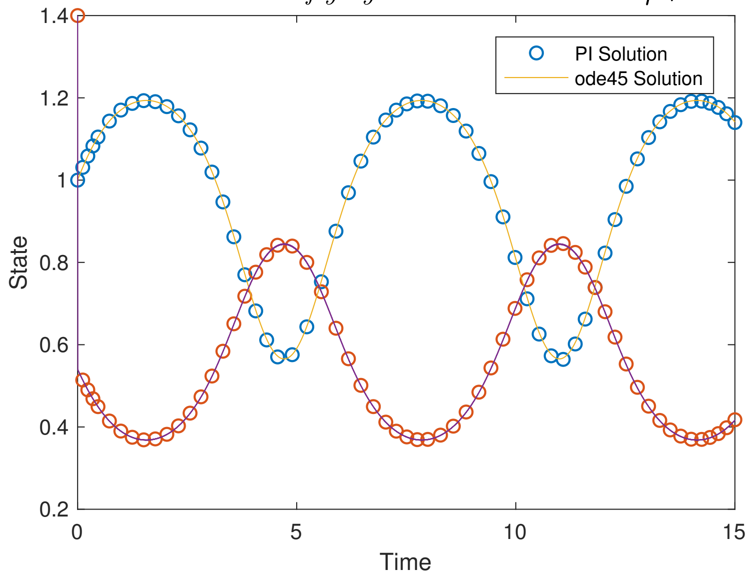
```
if ~exist('OCTAVE_VERSION','builtin')
    macInt='ode45'; else macInt='odeOct'; end
tic
[ts,xs,tms,xms] = PIG(macInt,microBurst,tSpan,x0);
secsPIGusingODEasMacro = toc
tic
[tClassic,xClassic] = feval(macInt,dxdt,tSpan,x0);
secsODEalone = toc
```

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

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

figure
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/lsode`.




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

Figure 2.9 plots the output.

- The problem may be made more stiff or less stiff by changing the time-scale separation parameter $\epsilon =$ `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.

```
clear all, close all
```

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

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

```
epsilon = 0.01;
dxdt=@(t,x) [ cos(x(1))*sin(x(2))*cos(t)
              (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.

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

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

```
x0 = [1 0];
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.

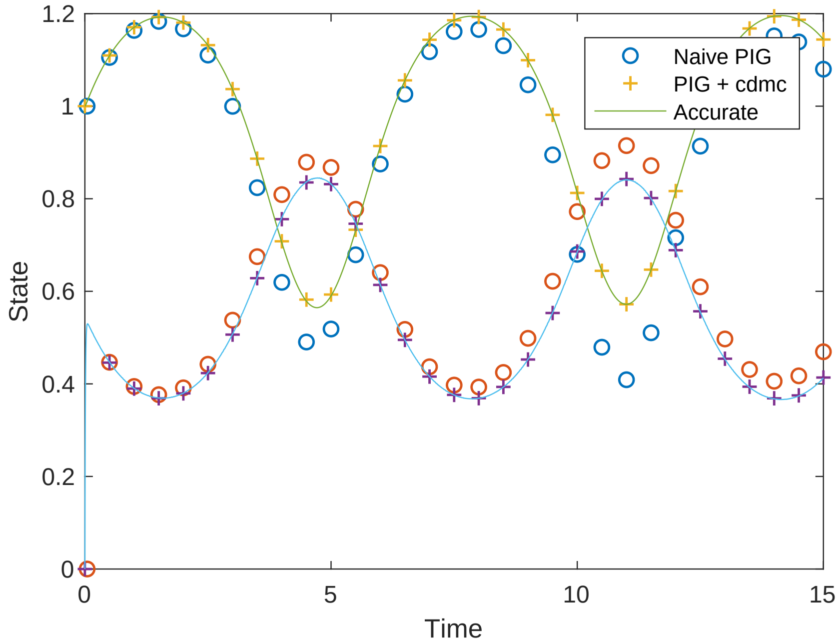
```
if ~exist('OCTAVE_VERSION','builtin')
    macInt='ode45'; else macInt='odeOct'; end
[nt,nx] = PIG(macInt,microBurst,tSpan,x0,[],[],'no cdmc');
[ct,cx] = PIG(macInt,microBurst,tSpan,x0);
[tClassic,xClassic] = feval(macInt,dxdt,tSpan,x0);
```

Figure 2.10 plots the output.

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

Chapter contents

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 2016*b*).

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.

Patch scheme for spatio-temporal dynamics

Setup problem and construct patches
Invoke `configpatches1` (for 1D) or `configpatches2` (for 2D) or `configpatches3` (for 3D) to setup the microscale problem (PDE, domain, boundary conditions, etc) and the desired patch structure (number of patches, patch size, coupling order, etc). These initialise the global struct `patches` that contains information required to simulate the microscale dynamics within each patch. If necessary, define additional components for the struct `patches` (e.g., see `homogenisationExample.m`).

Simulate the multiscale system
Generally invoke a PDE integrator to simulate the multiscale system of a user's microscale code within spatially separated patches. This integrator may be MATLAB/Octave defined (e.g., `ode23/ode45`) or user defined (e.g., a projective integrator). Input to the integrator is the function `patchSys1` (for 1D) or `patchSys2` (for 2D) or `patchSys3` (for 3D) which interfaces to the microscale's code. Other inputs are the macro-time span and initial conditions. Output from the integrator is the solution field over the given time span, but only within the defined patches.

Interface to microscale
`patchSys1/2/3` interfaces with the microscale PDE/lattice system and invokes the patch coupling conditions. Input is the field in every patch at one time-step, and output is time-derivatives of the field, or values at the next time-step, as appropriate.

Coupling conditions
`patchEdgeInt1/2/3` (for 1D, 2D, or 3D respectively) couple patches together by setting edge-values via macroscale interpolation of order in global `patches.ordCC`.

Microscale system
A user's microscale code, pointed to by `patches.fun`, codes the microscale dynamics on the interior of the patch microgrids, `patches.x`, to compute either a micro-step or time-derivatives.

Process results and plot

3.1 `configPatches1()`: configure spatial patches in 1D

Section contents

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.

```
function patches = configPatches1(fun,Xlim,Dom ...
    ,nPatch,ordCC,dx,nSubP,varargin)
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 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]

```
if nargout==0, global patches, end
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 ith microscale grid point in the Ith 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

```
if nargin==0
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.

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

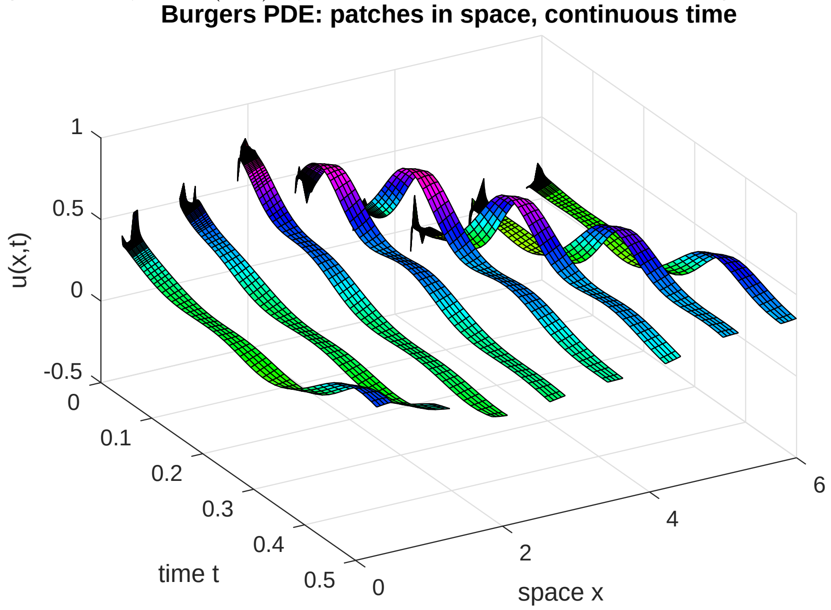
Set some initial condition, with some microscale randomness.

```
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).

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

Figure 3.2: field $u(x,t)$ of the patch scheme applied to Burgers' PDE.



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.

```
figure(1),clf
if 1, patches.x([1 end],:,:,:)=nan;  us=us.';
else us=reshape(patchEdgyInt1(us.'),[],length(ts));
end
mesh(ts,patches.x(:),us)
view(60,40), colormap(0.7*hsv)
title('Burgers PDE: patches in space, continuous time')
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.

```
ifOurCf2eps(mfilename)
return
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()).

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

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

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

3.1.2 Parse input arguments and defaults

```
p = inputParser;
fnValidation = @(f) isa(f, 'function_handle'); %test for fn name
addRequired(p,'fun',fnValidation);
addRequired(p,'Xlim',@isnumeric);
%addRequired(p,'Dom'); % nothing yet decided
addRequired(p,'nPatch',@isnumeric);
addRequired(p,'ordCC',@isnumeric);
addRequired(p,'dx',@isnumeric);
addRequired(p,'nSubP',@isnumeric);
addParameter(p,'nEdge',1,@isnumeric);
addParameter(p,'EdgyInt',false,@islogical);
addParameter(p,'nEnsem',1,@isnumeric);
addParameter(p,'hetCoeffs',[],@isnumeric);
addParameter(p,'parallel',false,@islogical);
addParameter(p,'nCore',1,@isnumeric);
parse(p,fun,Xlim,nPatch,ordCC,dx,nSubP,varargin{:});
```

Set the optional parameters.

```
patches.nEdge = p.Results.nEdge;
patches.EdgyInt = p.Results.EdgyInt;
patches.nEnsem = p.Results.nEnsem;
cs = p.Results.hetCoeffs;
patches.parallel = p.Results.parallel;
patches.nCore = p.Results.nCore;
```

Check parameters.

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

```
      ,'nSubP must be integer multiple of nEdge')
if ~patches.EdgyInt, assert(rem(nSubP/patches.nEdge,2)==1 ...
      ,'for non-edgyInt, nSubP/nEdge must be odd integer')
      end
if (patches.nEnsem>1)&(patches.nEdge>1)
      warning('not yet tested when both nEnsem and nEdge non-one')
      end
if patches.nCore>1
    warning('nCore>1 not yet tested in this version')
    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.

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

Default macroscale conditions are periodic with evenly spaced patches.

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

```
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.

```
patches.periodic=false;
switch Dom.type
case 'periodic'
    patches.periodic=true;
    if isfield(Dom,'bcOffset')
    warning('bcOffset not available for Dom.type = periodic'), end
    if isfield(Dom,'X')
    warning('X not available for Dom.type = periodic'), end
case {'equispace','chebyshev'}
    if ~isfield(Dom,'bcOffset'), Dom.bcOffset=[0;0]; end
    if length(Dom.bcOffset)==1
        Dom.bcOffset=repmat(Dom.bcOffset,2,1); end
    if isfield(Dom,'X')
    warning('X not available for Dom.type = equispace or chebyshev')
    end
case 'usergiven'
    if isfield(Dom,'bcOffset')
    warning('bcOffset not available for usergiven Dom.type'), end
    assert(isfield(Dom,'X'),'X required for Dom.type = usergiven')
otherwise
    error([Dom.type ' is unknown Dom.type'])
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.

```
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.

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

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

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

Check for staggered grid and periodic case.

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

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

```
switch Dom.type
```

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

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

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

```
  if ordCC>0
    [Cwtsr,Cwtsl] = patchCwts(ratio,ordCC,patches.stag);
    patches.Cwtsr = Cwtsr;  patches.Cwtsl = Cwtsl;
  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.

```
case 'equispace'
  X=linspace(Xlim(1)+((nSubP-1)/2-Dom.bcOffset(1))*dx ...
            ,Xlim(2)-((nSubP-1)/2-Dom.bcOffset(2))*dx ,nPatch);
  DX=diff(X(1:2));
  width=(1+patches.EdgyInt)/2*(nSubP-1-patches.EdgyInt)*dx;
  if DX<width*0.999999
     warning('too many equispace patches (double overlapping)')
     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]

```
case 'chebyshev'
  halfWidth=dx*(nSubP-1)/2;
  X1 = Xlim(1)+halfWidth-Dom.bcOffset(1)*dx;
  X2 = Xlim(2)-halfWidth+Dom.bcOffset(2)*dx;
%  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.

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

Assign the centre-patch coordinates.

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

```
case 'usergiven'
  X = reshape(Dom.X,1,[]);
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).

```
xs = dx*( (1:nSubP)-mean(1:nSubP) );
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()`.

```
nE = patches.nEnsem;
patches.le = 1:nE;
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.

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

```
  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.

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

```
        patches.cs(:,:,i) = cs(is,:);
    end
    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.

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

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

End the two if-statements.

```
  end%if-else nEnsem>1
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]

```
if patches.parallel
%  theparpool=gcp()
  spmd
```

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

```
  pari = 1;
  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.

```
  switch pari
    case 1, patches.x=codistributed(patches.x,patches.codist);
  otherwise
    error('should never have bad index for parallel distribution')
  end%switch
  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.

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

Fin

```
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.

```
function dudt=patchSys1(t,u,patches,varargin)
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`×`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` × 1 × 1 × `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()`.

```
sizeu = size(u);
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.

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

```
dudt([1:n end-n+1:end],:,:,:) = 0;
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`.

```
function u=patchEdgeInt1(u,patches)
if nargin<2, global patches, end
```

Input

- `u` is a vector/array of length `nSubP` $\cdot$ `nVars` $\cdot$ `nEnsem` $\cdot$ `nPatch` where there are `nVars`$\cdot$`nEnsem` field values at each of the points in the `nSubP`$\times$`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.

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

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

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

```
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.

```
x = patches.x;
if patches.nEdge>1
  nEdge = patches.nEdge;
  x = x(1:nEdge:nx,:,:,:);
  nx = nx/nEdge;
  u = reshape(u,nEdge,nx,nVars,nEnsem,Nx);
  nVars = nVars*nEdge;
  u = reshape( permute(u,[2 1 3:5]) ,nx,nVars,nEnsem,Nx);
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).

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

3.3.1 Periodic macroscale interpolation schemes

```
if patches.periodic
```

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

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

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

```
szUxO=size(Ux);
szUxO=[szUxO ones(1,4-length(szUxO)) 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.

```
  if patches.parallel
    dmu = zeros(szUxO,patches.codist); % 5D
  else
    dmu = zeros(szUxO); % 5D
  end
```

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

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

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

```
for k = 3:patches.ordCC
  dmu(:,:,:,:,k) =       dmu(:,:,:,Ip,k-2) ...
    -2*dmu(:,:,:,I,k-2) +dmu(:,:,:,Im,k-2);
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`.

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

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

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

```
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 `Nx` patches we resolve 'wavenumbers' $|k| < \texttt{Nx}/2$, so set row vector $\texttt{ks} = k2\pi/N$ for 'wavenumbers' $k = (0\,,1\,,\ldots,k_{\max}\,,-k_{\max}\,,\ldots,-1)$ for odd N, and $k = (0\,,1\,,\ldots,k_{\max}\,,(k_{\max}+1)\,,-k_{\max}\,,\ldots,-1)$ 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]

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

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

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

```
if ~patches.EdgyInt
  Cleft = fft(u(i0  ,:,:,:),[],4);
  Cright = Cleft;
else
  Cleft = fft(u(2   ,:,:,:),[],4);
  Cright= fft(u(nx-1,:,:,:),[],4);
end
```

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

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

```
if patches.stag
 nVars = nVars/2;
 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.

```
  Nx = 2*Nx;
  v(:,:,:,1:2:Nx) = u(:,:,1,:,:);
  v(:,:,:,2:2:Nx) = u(:,:,2,:,:);
  u = v;
end%if patches.stag
end%if patches.ordCC
```

3.3.2 Non-periodic macroscale interpolation

```
else% patches.periodic false
assert(~patches.stag, ...
'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.

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

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

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

```
for q = 1:p
  i = 1:Nx-q;
  F(:,:,:,i,q+1) = (F(:,:,:,i+1,q)-F(:,:,:,i,q)) ...
                 ./(X(:,:,:,i+q)  -X(:,:,:,i));
end
```

Now interpolate to the edge-values at locations Xedge.

```
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??

```
if true
  i = max(1,min(1:Nx,Nx-ceil(p/2))-floor(p/2));
  Uedge = F(:,:,:,i,p+1);
  for q = p:-1:1
    Uedge = F(:,:,:,i,q)+(Xedge-X(:,:,:,i+q-1)).*Uedge;
  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]

```
else%if false
  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.

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

Initialise to highest divide difference, surrounded by zeros.

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

Complete Horner evaluation of the relevant polynomials.

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

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

```
u(1 ,:,patches.le,I) = Uedge(1,:,:,I);
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`.

```
if isfield(patches,'intTest')&&patches.intTest
else % usual case
  u( 1,:,:, 1) = nan;
  u(nx,:,:,Nx) = nan;
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.

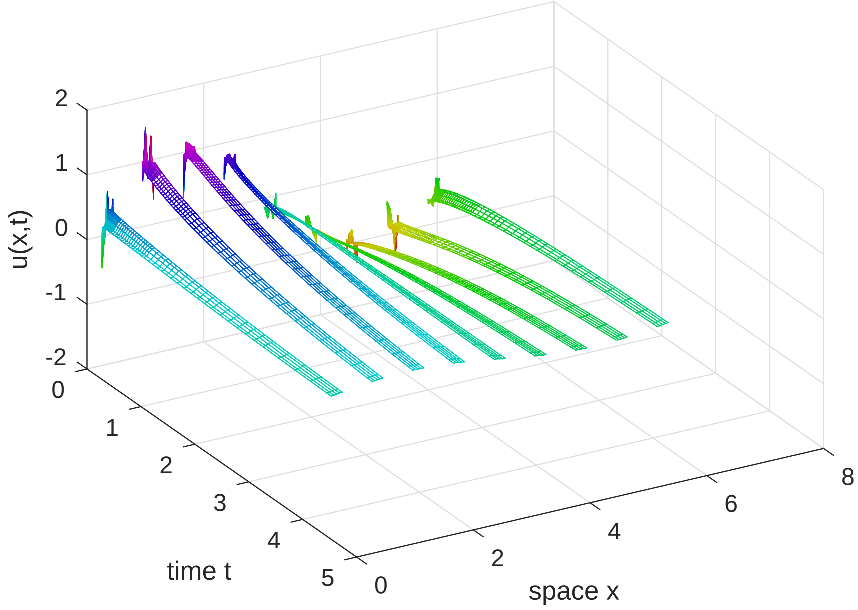
```
end%if patches.periodic
```

Unfold multiple edges No need to restore x.

```
if patches.nEdge>1
  nVars = nVars/nEdge;
  u = reshape( u ,nx,nEdge,nVars,nEnsem,Nx);
  nx = nx*nEdge;
  u = reshape( permute(u,[2 1 3:5]) ,nx,nVars,nEnsem,Nx);
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

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

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

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).

```
mPeriod = 3
cDiff = exp(randn(mPeriod,1))
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.

```
global patches
nPatch = 9
ratio = 0.2
nSubP = 2*mPeriod+1
Len = 2*pi;
ordCC = 4;
configPatches1(@heteroDiff,[0 Len],nan,nPatch ...
    ,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.

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

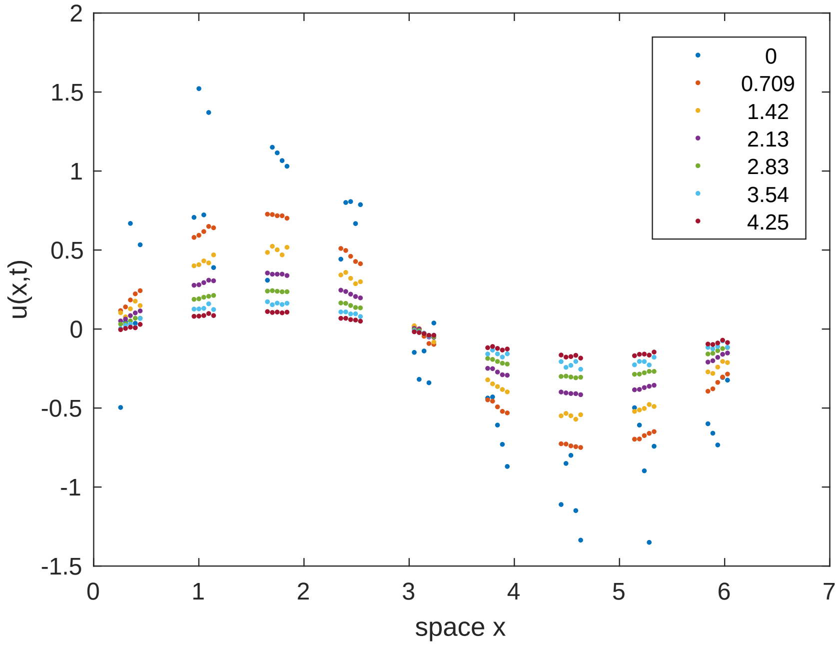
Plot the simulation in Figure 3.3.

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

The code may invoke this integration interface.

```
function [ts,xs] = odeOcts(dxdt,tSpan,x0)
    if length(tSpan)>2, ts = tSpan;
    else ts = linspace(tSpan(1),tSpan(end),21)';
    end
    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.




```
    xs = lsode(@(x,t) dxdt(t,x),x0,ts);
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`.

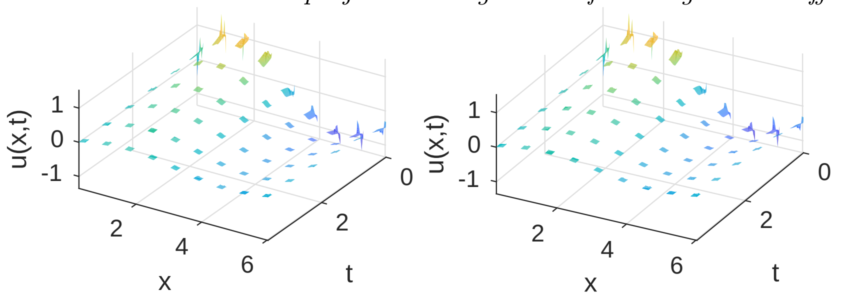
1. configPatches1 (done in first part)
2. PIRK2 $\mapsto$ heteroBurst $\mapsto$ micro-integrator $\mapsto$ patchSys1 $\mapsto$ heteroDiff
3. process results

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

```
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.




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

Plot the macroscale predictions to draw Figure 3.4.

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

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

```
figure(3),clf
for k = 1:2, subplot(2,2,k)
  surf(tss,xs(:),uss',  'EdgeColor','none')
  ylabel('$x$'), xlabel('$t$'), zlabel('$u(x,t)$')
  axis tight, view(126-4*k,45)
end
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`.

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

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

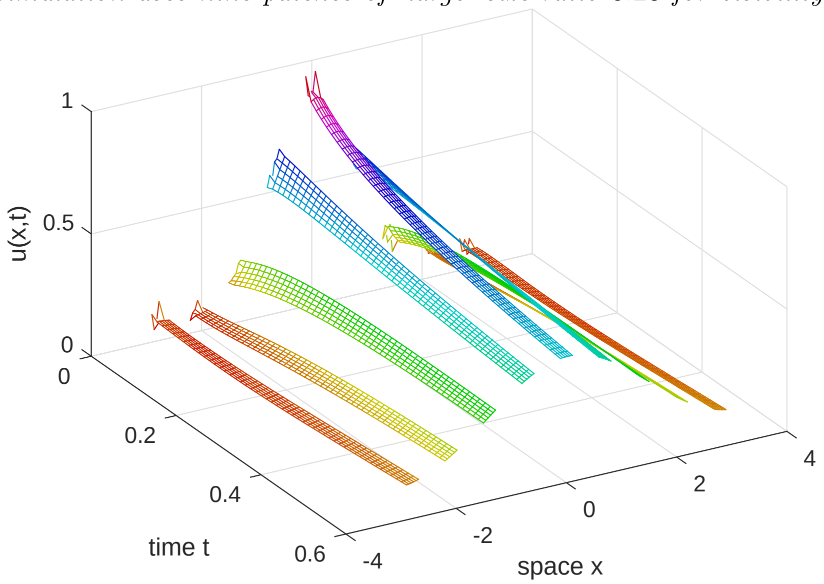
3.4.3 heteroBurst(): a burst of heterogeneous diffusion

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.

```
function [ts, ucts] = heteroBurst(ti, ui, bT)
        if ~exist('OCTAVE_VERSION','builtin')
        [ts,ucts] = ode23( @patchSys1,[ti ti+bT],ui(:));
        else % octave version
        [ts,ucts] = rk2Int(@patchSys1,[ti ti+bT],ui(:));
        end
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

$$\frac{\partial u_i}{\partial t} = \frac{1}{dx^2}\delta[c_{i-1/2}\delta u_i], \tag{3.2}$$

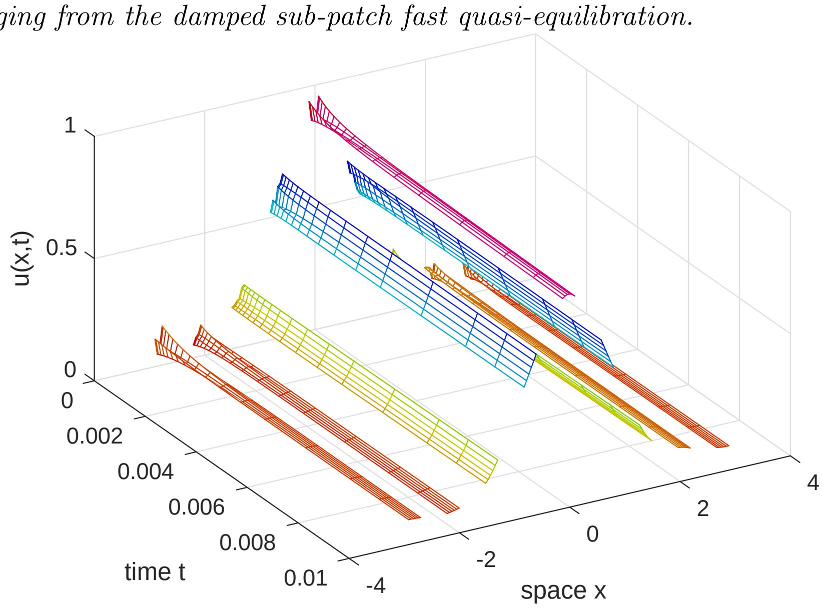
in terms of the centred difference operator δ. The system has a microscale heterogeneity via the coefficients $c_{i+1/2}$ which we assume to have some given known periodicity. Figure 3.6 shows one patch simulation of this system: observe the effects of the heterogeneity within each patch.

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 $0, 1, 2, \ldots$. Then the heterogeneity is repeated to fill each patch, and phase-shifted for an ensemble.

```
mPeriod = 3%randi([2 5])
% set random diffusion coefficients
cHetr=exp(0.3*randn(mPeriod,1));
%cHetr = [3.966;2.531;0.838;0.331;7.276];
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.EdgyInt` 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.

```
global patches
nPatch = 9
ratio = 0.25;
```

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

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

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

Integrate using standard integrators.

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

Plot space-time surface of the simulation We want to see the edge values of the patches, so we adjoin a row of `nan`s in between patches. For the field values (which are rows in `us`) we need to reshape, permute, interpolate to get edge values, pad with `nan`s, and reshape again. In the case of an ensemble of phase-shifts, we plot the mean over the ensemble.

```
xs = squeeze(patches.x);
us = patchEdgeInt1( permute( reshape(us ...
    ,length(ts),nSubP,nEnsem,nPatch) ,[2 1 3 4]) );
ustd = squeeze(std(us,0,3));
us = squeeze(mean(us,3));
if 0, % omit interpolated edges
    us([1 end],:,:) = nan;
    ustd([1 end],:,:) = nan;
else % insert nans between patches
    xs(end+1,:) = nan;
    us(end+1,:,:) = nan;
    ustd(end+1,:,:) = nan;
end
us=reshape(permute(us,[1 3 2]),[],length(ts));
ustd=reshape(permute(ustd,[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.

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

```
  case 2, [~,j]=min(abs(ts(:)-linspace(ts(1),ts(end),50)));
  end
  figure(p),clf
  mesh(ts(j),xs(:),us(:,j))
  view(60,40), colormap(0.8*hsv)
  xlabel('time $t$'), ylabel('space $x$'), zlabel('$u(x,t)$')
  ifOurCf2eps([mfilename 'U' num2str(p)])
end
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.

```
nPatch = 13
ratio = 0.01;

leadingEvals=[];
for ord=0:2:8
  ordInterp=ord
  configPatches1(@heteroDiff,[-pi pi],nan,nPatch ...
      ,ord,ratio,nSubP,'EdgyInt',true,'nEnsem',nEnsem ...
    ,'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.

```
  u0 = zeros(nSubP,1,nEnsem,nPatch);
  u0([1 end],:,:,:)=nan; u0=u0(:);
  i=find(~isnan(u0));
  nJ=length(i);
  Jac=nan(nJ);
  for j=1:nJ
    u0(i)=((1:nJ)==j);
    dudt=patchSys1(0,u0);
    Jac(:,j)=dudt(i);
  end
  nonSymmetric=norm(Jac-Jac')
  assert(nonSymmetric<5e-9,'failed symmetry')
  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
```

```
  [evecs,evals]=eig(Jac);
  eval=-sort(-diag(real(evals)));
  nZeroEv=sum(eval(:)>-1e-5)
  leadingEvals=[leadingEvals eval(1:3*nPatch)];
%  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.

```
end
disp('     spectral    quadratic      quartic  sixth-order  ...')
leadingEvals=leadingEvals
```

End of the main script.

3.5.2 `heteroDiff()`: heterogeneous diffusion

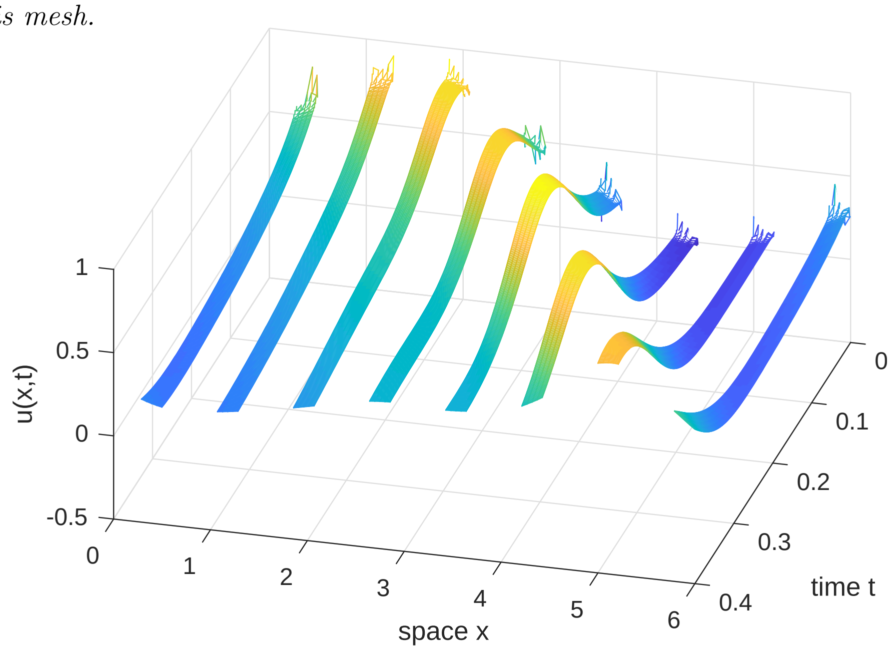
This function codes the lattice heterogeneous diffusion inside the patches. For 2D input arrays `u` and `x` (via edge-value interpolation of `patchSys1`, Section 3.2), computes the time derivative (3.1) at each point in the interior of a patch, output in `ut`. The column vector of diffusivities c_i,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

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

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

Section contents

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.

```
global patches
nPatch = 8
ratio = 0.2
nSubP = 7
interpOrd = 4
Len = 2*pi
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).

```
u0 = 0.4*(1+sin(patches.x))+0.1*randn(size(patches.x));
[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.

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

Save the plot to file to form Figure 3.8.

```
ifOurCf2eps([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.

```
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.

```
ts = linspace(0,0.5,11);
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.

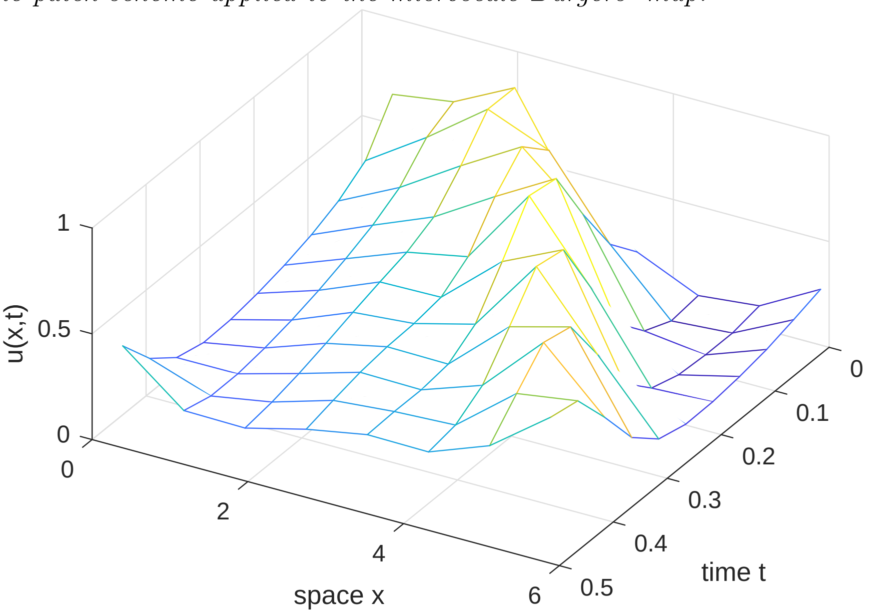
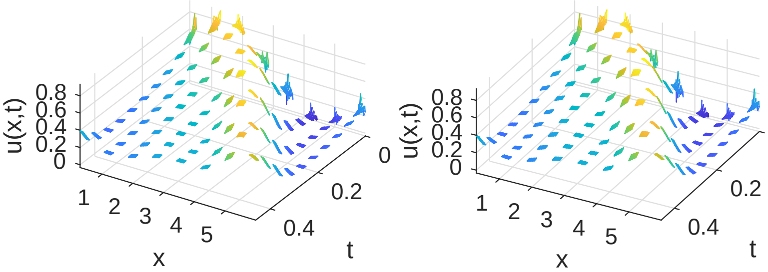


Figure 3.10: the microscale field $u(x,t)$ during each of the microscale bursts used in the projective integration. View this stereo pair cross-eyed.




```
addpath('../ProjInt')
[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.

```
figure(2),clf
midP = (nSubP+1)/2;
mesh(ts,xs(midP,:),us(:,midP:nSubP:end)')
xlabel('time $t$'), ylabel('space $x$'), zlabel('$u(x,t)$')
view(120,50)
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.

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

```
  mesh(tss,xs(:),uss')
  ylabel('space $x$'),xlabel('time $t$'),zlabel('$u(x,t)$')
  axis tight, view(126-4*k,50)
end
ifOurCf2eps([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).

```
function u = burgersMap(t,u,patches)
  u = squeeze(u);
  dx = diff(patches.x(2:3));
  dt = dx^2/2;
  i = 2:size(u,1)-1;
  u(i,:) = u(i,:) +dt*( diff(u,2)/dx^2 ...
      -20*u(i,:).*(u(i+1,:)-u(i-1,:))/(2*dx) );
end
```

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

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

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

```
  global patches
  dt = diff(patches.x(2:3))^2/2;
  ndt = ceil(bT/dt -0.2);
  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.

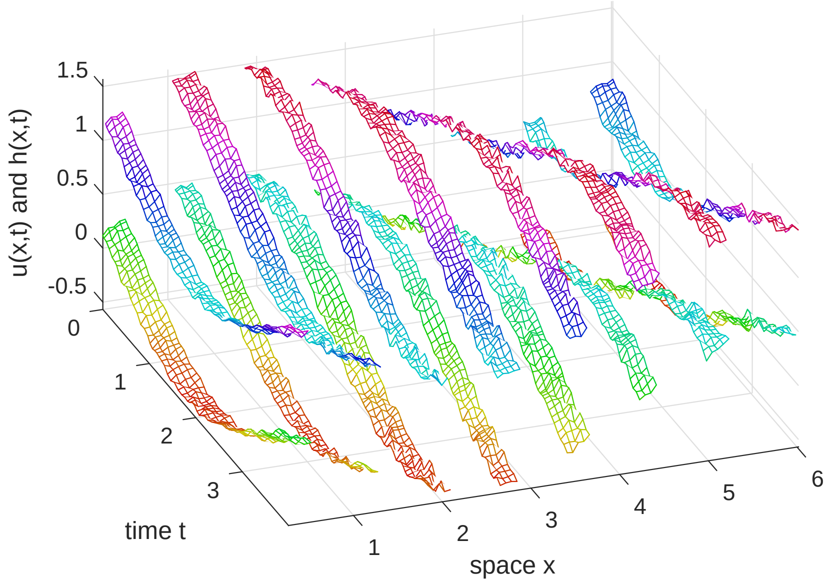
```
  us = nan(ndt+1,numel(ui));
  us(1,:) = reshape(ui,1,[]);
  for j = 1:ndt
    ui = patchSys1(ts(j),ui);
    us(j+1,:) = reshape(ui,1,[]);
  end
```

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

```
  ts(ndt+1) = ti+bT;
  us(ndt+1,:) = us(ndt,:) ...
    + diff(ts(ndt:ndt+1))/dt*diff(us(ndt:ndt+1,:));
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

Section contents

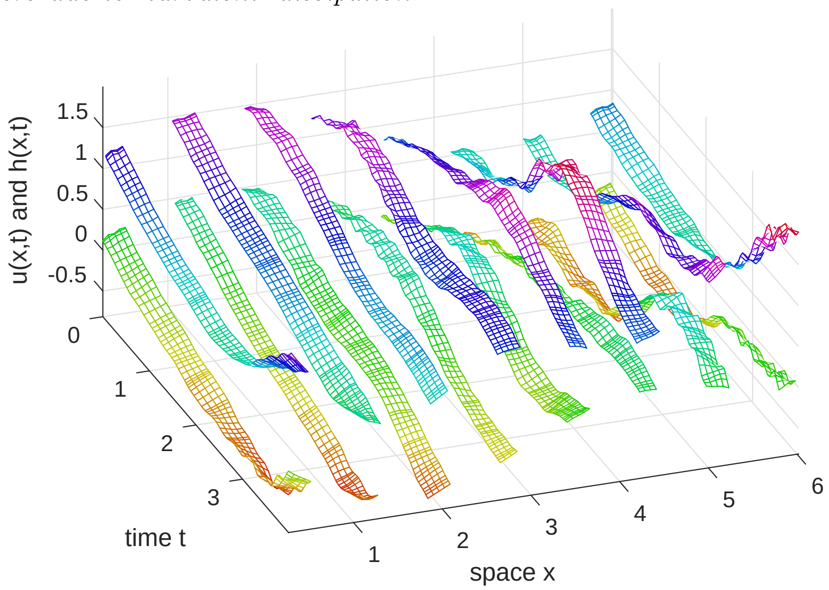
Figure 3.11 shows an example simulation in time generated by the patch scheme applied to an ideal wave PDE (Cao & Roberts 2013). The inter-patch coupling is realised by spectral interpolation of the mid-patch values to the patch edges.

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, 2016*a*).

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

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

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, 2016*a*, 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 (2016*b*) 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.

```
global patches
nPatch = 8
ratio = 0.2
nSubP = 11 %of the form 4*n-1
Len = 2*pi;
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.

```
uPts = mod( (1:nSubP)'+(1:nPatch) ,2);
hPts = find(uPts==0);
uPts = find(uPts==1);
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).

```
U0 = nan(nSubP,nPatch);
U0(hPts) = 1+0.5*sin(patches.x(hPts));
U0(uPts) = 0+0.5*sin(patches.x(uPts));
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.

```
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.

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

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

Plot the simulation.

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

Optionally save the plot to file.

```
ifOurCf2eps([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.

```
  patches.fun = @waterWavePDE;
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.

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

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

```
  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.

```
  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.

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

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

```
  Ut(patches.hPts) = ht(patches.hPts);
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()`.

```
function Ut = waterWavePDE(t,U,patches)
  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.

```
  dx = diff(patches.x(2:3));
  U = squeeze(U);
  Ut = nan(size(U));  ht = Ut;
  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.

```
  ii = i(2:end-1);
  V = Ut;
  V(ii,:) = (U(ii+1,:)+U(ii-1,:))/2;
  V(1:2,:) = 2*U(2:3,:)-V(3:4,:);
  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.

```
  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 $\texttt{U}_i$ and $\texttt{V}_{i\pm1}$; and h-values in $\texttt{V}_i$ and $\texttt{U}_{i\pm1}$.

```
  Ut(i,:) = -0.985*(U(i+1,:)-U(i-1,:))/(2*dx) ...
    -0.003*U(i,:).*rabs(U(i,:)./V(i,:)) ...
    -1.045*U(i,:).*(V(i+1,:)-V(i-1,:))/(2*dx) ...
    +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:

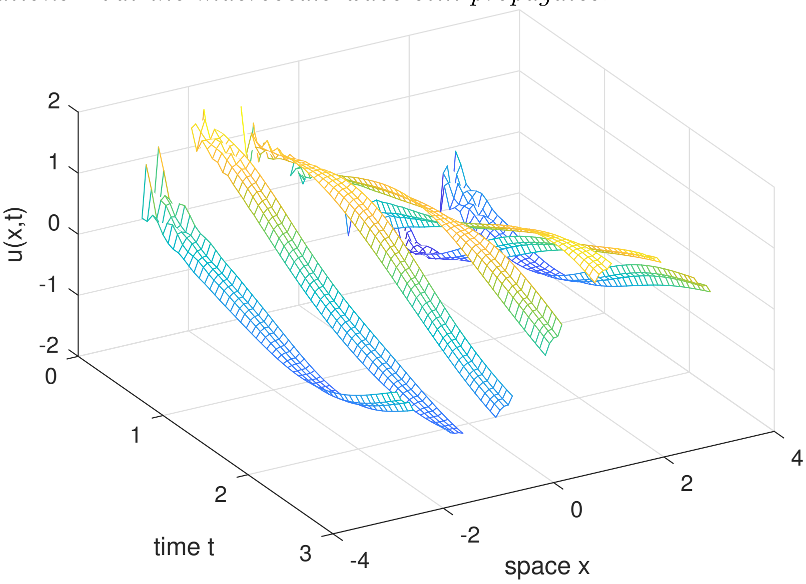
$$\begin{aligned} u_{xx} &\approx \frac{1}{4\delta^2}(u_{i-2} - 2u_i + u_{i+2}) \\ &= \frac{1}{4\delta^2}(u_{i-2} + u_i - 4u_i + u_i + u_{i+2}) \\ &= \frac{1}{2\delta^2}\left(\frac{u_{i-2} + u_i}{2} - 2u_i + \frac{u_i + u_{i+2}}{2}\right) \\ &= \frac{1}{2\delta^2}\left(\bar u_{i-1} - 2u_i + \bar u_{i+1}\right).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

Then overwrite the unwanted $\dot u_{ij}$ with the corresponding wanted $\dot h_{ij}$.

```
  Ut(patches.hPts) = ht(patches.hPts);
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

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

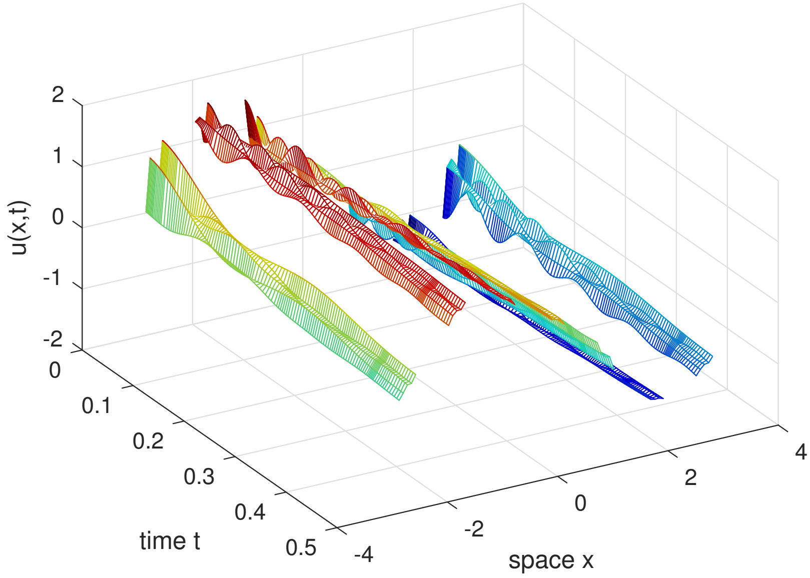
in terms of the centred difference operator δ. The system has a microscale heterogeneity via the coefficients $c_{i+1/2}$ which we assume to have some given known periodicity. Figure 3.13 shows one patch simulation of this system: observe the effects of the heterogeneity within each patch.

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, $1, 2, 3, \ldots$. Then the heterogeneity is to be repeated `nPeriodsPatch` times within each patch.

```
mPeriod = 3
cHetr = exp(1*randn(mPeriod,1));
cHetr = cHetr*mean(1./cHetr) % normalise
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.EdgyInt` to one means the edge-values come from interpolating the opposite next-to-edge values of the patches (not the mid-patch values).

```
global patches
nPatch = 7
ratio = 0.25
nSubP = nPeriodsPatch*mPeriod+2
configPatches1(@heteroWave,[-pi pi],nan,nPatch ...
    ,0,ratio,nSubP,'EdgyInt',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`.

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

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

Plot space-time surface of the simulation We want to see the edge values of the patches, so we adjoin a row of `nan`s in between patches. For the field values (which are rows in `us`) we need to reshape, permute, interpolate to get edge values, pad with `nan`s, and reshape again.

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

```
for p=1:2
  switch p
  case 1, j=find(ts<0.5);
  case 2, [~,j]=min(abs(ts-linspace(ts(1),ts(end),50)));
  end
  figure(p),clf
  mesh(ts(j),xs(:),squeeze(us(:,1,j))),  view(60,40)
  xlabel('time $t$'), ylabel('space $x$'), zlabel('$u(x,t)$')
  ifOurCf2eps([mfilename 'U' num2str(p)])
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.

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

```
for j=1:nJ
   u0(i)=((1:nJ)==j);
   dudt=patchSys1(0,u0);
   Jac(:,j)=dudt(i);
end
Jac(abs(Jac)<1e-12)=0;
```

Find the eigenvalues of the Jacobian, and list for inspection in Table 3.2.

```
[evecs,evals]=eig(Jac);
eval=sort(diag(evals));
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 `u` (u_{ij} = `u(i,1,j)` and v_{ij} = `u(i,2,j)`) and 2D array `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 `ut`:

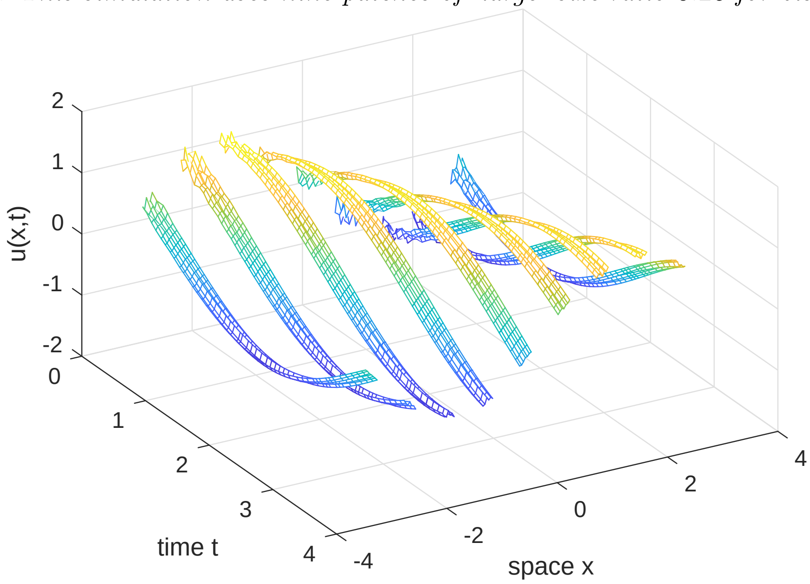
$$\frac{\partial u_{ij}}{\partial t} = v_{ij}\,, \quad \frac{\partial v_{ij}}{\partial t} = \frac{1}{dx^2}\delta[c_{i-1/2}\delta u_{ij}] + \frac{0.02}{dx^2}\delta^2 v_{ij}\,.$$

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

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

Section contents

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

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

Figure 3.15 shows one patch simulation of this space-time system, except it also includes a $\nu = 0.001$ small 'viscous' dissipation, $\nu\delta^2 u_i/d^2$, 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 $\mapsto$ patchSys1 $\mapsto$ 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, $0, 1, 2, \ldots$—except that the normalisation is exact only for periods 3 and 5. Then the heterogeneity is repeated `nPeriodsPatch` times within each patch.

```
mPeriod = 5 % needs to be odd for a wave
cHetr = exp(0.1*randn(mPeriod,1)); % 0.3 appears max reasonable
if mPeriod==3,
    cHetr=cHetr*mean(cHetr.^2)/prod(cHetr) % normalise
elseif mPeriod==5,
    cHetr=cHetr*mean(cHetr.^2.*cHetr([3 4 5 1 2]).^2)/prod(cHetr)
else cHetr=cHetr*mean(1./cHetr) % roughly normalise
end
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.

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

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

```
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`.

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

Integrate using standard stiff integrators.

```
if ~exist('OCTAVE_VERSION','builtin')
    [ts,us] = ode23(@patchSys1, [0 3.5], u0(:));
else % octave version
    [ts,us] = odeOcts(@patchSys1, [0 0.5], u0(:));
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 `nan`s, and reshape again.

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

```
[~,j]=min(abs(ts-linspace(ts(1),ts(end),50)));
figure(1),clf
mesh(ts(j),xs(:),us(:,j)),  view(60,40)
xlabel('time $t$'), ylabel('space $x$'), zlabel('$u(x,t)$')
ifOurCf2eps([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).

```
ratio=0.01
nPatch=19
leadingFreqs=[];
for ord=0:2:8
    ordInterp=ord
    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
```

```
        ,ratio,nSubP,'EdgyInt',EdgyInt,'hetCoeffs',cHetr);
    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.

```
    u0=0*patches.x; u0([1 end],:)=nan; u0=u0(:);
    i=find(~isnan(u0));
    nJ=length(i);
    Jac=nan(nJ);
    for j=1:nJ
       u0(i)=((1:nJ)==j);
       dudt=patchSys1(0,u0);
       Jac(:,j)=dudt(i);
    end
    nonSkewSymmetric=norm(Jac+Jac')
    assert(nonSkewSymmetric<1e-10,'failed skew-symmetry')
    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.

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

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

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

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

```
end
disp('     spectral    quadratic      quartic  sixth-order ...')
leadingFreqs = leadingFreqs
```

End of the main script.

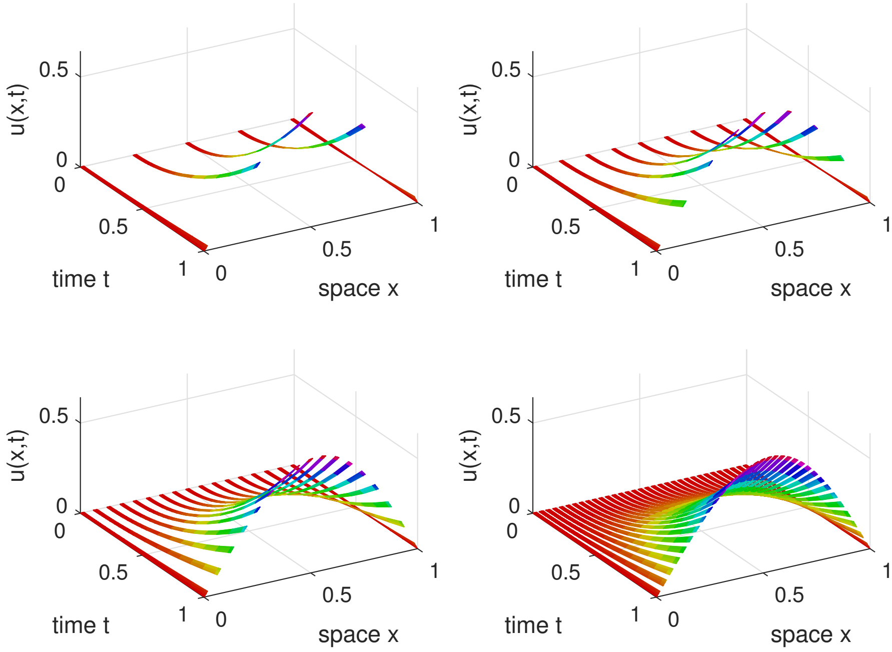
3.9.2 `waveFirst()`: first-order wave PDE

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`.

```
function ut = waveFirst(t,u,patches)
  u=squeeze(u);
  dx = diff(patches.x(2:3)); % space step
  i = 2:size(u,1)-1; % interior points in a patch
  ut = nan+u;        % preallocate output array
  ut(i,:) = -(patches.cs(i).*u(i+1,:) ...
              -patches.cs(i-1).*u(i-1,:))/(2*dx) ...
             +patches.nu*diff(u,2)/dx^2;
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

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

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.

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

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

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

Loop to explore errors on various sized patches.

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

Determine indices of patches that are common in various resolutions

```
    if isnan(I), I=1:nP; else I=2*I-1; end
```

Establish the global data struct `patches` for the microscale heterogeneous lattice diffusion system (3.7) solved on domain $[0, 1]$, with `nP` patches, and say fourth order interpolation to provide the edge-values. Setting `patches.EdgyInt` true means the edge-values come from interpolating the opposite next-to-edge values of the patches (not the mid-patch values).

```
    global patches
    ordCC = 4
    configPatches1(@heteroDiffF,[0 1],'equispace',nP ...
        ,ordCC,dx,nSubP,'EdgyInt',true,'hetCoeffs',a);
    DX = mean(diff(squeeze(patches.x(1,1,1,:))))
    DXs=[DXs;DX];
```

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

```
if 0 % given forcing is exact
  patches.f1=2*( patches.x-patches.x.^2 );
  patches.f2=2*0.5+0*patches.x;
else% simple exp.sine forcing
  patches.f1=sin(pi*patches.x).*exp(patches.x);
  patches.f2=pi/2*sin(pi*patches.x).*exp(patches.x);
end%if
```

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

```
u0 = 0*patches.x;
tic
[ts,us] = ode15s(@patchSys1, [0 1], u0(:));
cpuTime=toc
```

Plot space-time surface of the simulation We want to see the edge values of the patches, so adjoin a row of nans in between patches. For the field values (which are rows in us) we need to reshape, permute, interpolate to get edge values, pad with nans, and reshape again.

```
xs = squeeze(patches.x);
us = patchEdgeInt1( permute( reshape(us ...
    ,length(ts),nSubP,1,nP) ,[2 1 3 4]) );
us = squeeze(us);
xs(end+1,:) = nan;  us(end+1,:,:) = nan;
uss=reshape(permute(us,[1 3 2]),[],length(ts));
```

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

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

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

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

```
    Xsp=Xs;
end%for log2Nx
ifOurCf2eps(mfilename) %optionally save plot
```

Assess errors by comparing to the full-domain solution

```
DXs=DXs
Uerr=squeeze(max(max(abs(Us-Us(:,:,end)))))
figure(2),clf,
loglog(DXs,Uerr,'o:')
xlabel('$H$'),ylabel('error')
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.

```
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.

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

Two basic parameters, and initialise result array to NaNs.

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

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

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

Code the microscale forced diffusion.

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

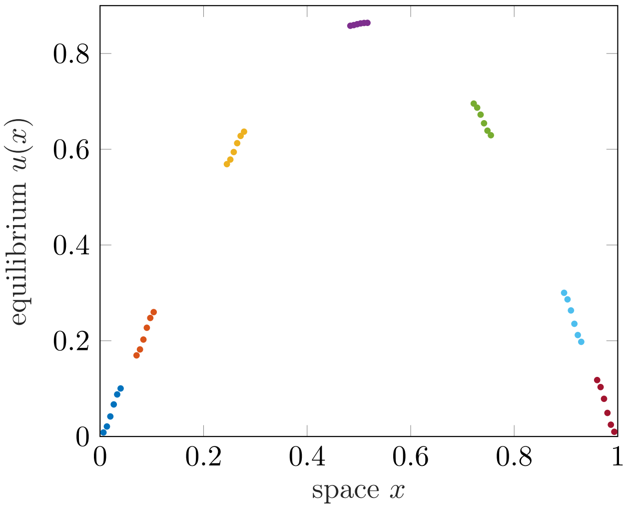


Figure 3.17: Equilibrium of the heterogeneous diffusion problem with forcing the same as that applied at time $t = 1$, and for relatively large $\epsilon = 0.04$ so we can see the patches. By default this code sets $\epsilon = 0.004$ whence the microscale heterogeneity and patches are tiny.

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].

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

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

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

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

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

```
if 0 % given forcing
  patches.f1 = 2*( patches.x-patches.x.^2 );
  patches.f2 = 2*0.5+0*patches.x;
else% simple exp-sine forcing
  patches.f1 = sin(pi*patches.x).*exp(patches.x);
  patches.f2 = pi/2*sin(pi*patches.x).*exp(patches.x);
end%if
```

Find equilibrium with fsolve We seek the equilibrium for the forcing that applies at time $t = 1$ (as if that specific forcing were applying for all time). 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.

```
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.

```
u([1 end],:,:,:) = nan;
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).

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

Plot the equilibrium see Figure 3.17.

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

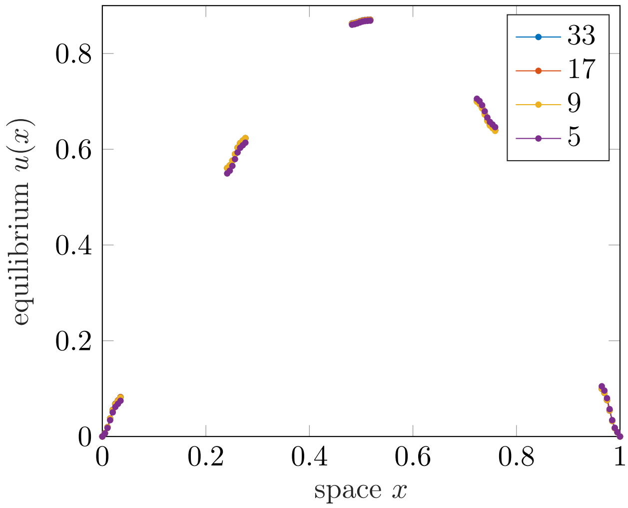


Figure 3.18: Equilibrium of the heterogeneous diffusion problem for relatively large $\epsilon = 0.03$ *so we can see the patches. The solution is obtained with various numbers of patches, but we only compare solutions in these five common patches.*

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

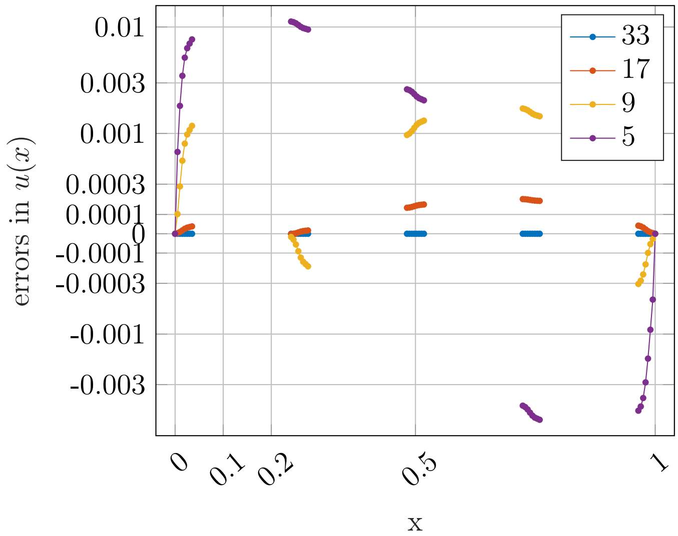


Figure 3.19: Errors in the equilibrium of the heterogeneous diffusion problem for relatively large $\epsilon = 0.03$. The solution is obtained with various numbers of patches, but we only plot the errors within these five common patches.

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).

```
clear all
global patches
%global OurCf2eps, OurCf2eps=true %option to save plots
switch 1
    case 1, Dom.type = 'equispace'
    case 2, Dom.type = 'chebyshev'
    case 3, Dom.type = 'usergiven'
    end% switch
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.

```
mPeriod = 6
z = (0.5:mPeriod)'/mPeriod;
a = 1./(2-cos(2*pi*z))
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 `log2Nmax` $= 129$ ($\epsilon = 0.008$) in a few seconds:

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

Set the periodicity ϵ, and other microscale parameters.

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

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

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

```
    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).

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

Configure the patches:

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

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

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

```
    if log2N==log2Nmax
      u0 = zeros(nSubP,1,1,nPatch);
    else u0 = u0(:,:,:,1:2:end);
    end
    u0([1 end],:) = nan;
    patches.i = find(~isnan(u0));
    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).

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

Store the solution into the patches, and give magnitudes—Inf norm is max(abs()).

```
    normSoln = norm(uSoln,Inf)
    normResidual = norm(resSoln,Inf)
    u0(patches.i) = uSoln;
    u0 = patchEdgeInt1(u0);
    u0( 1 ,:,:, 1 ) = 0;
    u0(end,:,:,end) = 0;
```

Concatenate the solution on common patches into stores.

```
    us=cat(3,us,squeeze(u0(:,:,:,Ps)));
    xs=cat(3,xs,squeeze(patches.x(:,:,:,Ps)));
    nPs = [nPs;nPatch];
```

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

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

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

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

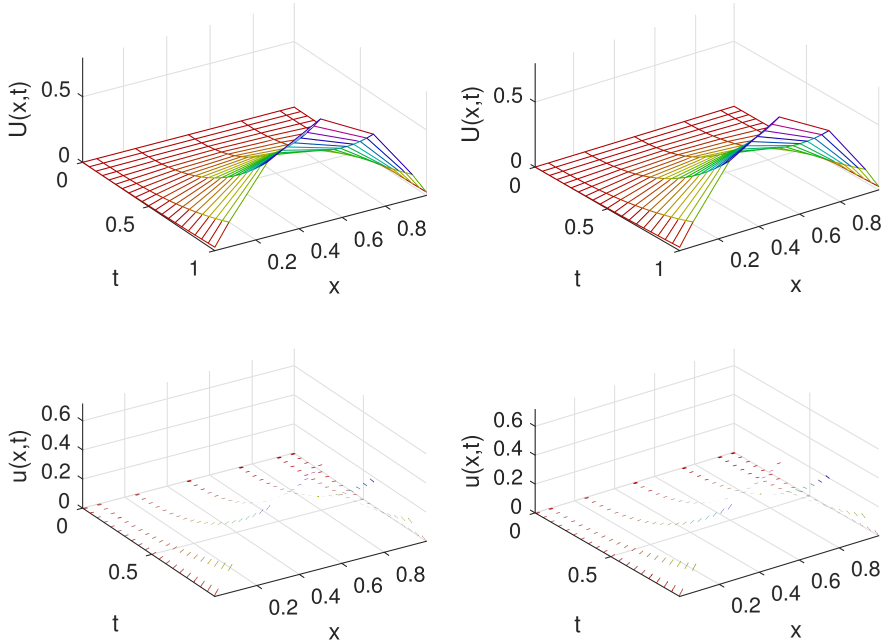
Reshape solution field.

```
figure(1),clf
plot(x(:),u,'.-'), legend(num2str(nPs))
xlabel('space $x$'),ylabel('equilibrium $u(x)$')
ifOurCf2tex([mfilename 'us'])%optionally save
```

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

```
err = u(:,1)-u;
figure(2), clf
plot(x(:),err,'.-'); legend(num2str(nPs))
quasiLogAxes(10,sqrt(prod(meanAbsErrs(2:3))))
xlabel('space $x$'), ylabel('errors in $u(x)$')
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

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

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.

```
clear all
%global OurCf2eps, OurCf2eps=true %option to save plots
mPeriod = 6
y = linspace(0,1,mPeriod+1)';
a = ( 3+cos(2*pi*y(1:mPeriod)) )/30
A0 = 1/mean(1./a) % roughly the effective diffusivity
```

The microscale diffusivity has an additional additive component of $+\frac{1}{30}\cos(2\pi t/\epsilon^2)$ which is coded into time derivative routine via global `microTimePeriod`.

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

```
nPeriodsPatch = 2 % any integer
rEpsilon = 100
dx = 1/(mPeriod*rEpsilon+1)
nSubP = nPeriodsPatch*mPeriod+2
tol=1e-9;
```

Set the time periodicity (global).

```
global microTimePeriod
microTimePeriod = 1/rEpsilon^2
```

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

```
nPatch = 7
ordCC = 4
```

```
Dom = 'chebyshev'
global patches
configPatches1(@heteroDiffF,[0 1],Dom,nPatch ...
    ,ordCC,dx,nSubP,'EdgyInt',true,'hetCoeffs',a);
DX = mean(diff(squeeze(patches.x(1,1,1,:))))
```

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

```
if 0 % given forcing
  patches.f1=2*( patches.x-patches.x.^2 );
  patches.f2=2*0.5+0*patches.x;
else% simple sine forcing
  patches.f1=sin(pi*patches.x);
  patches.f2=pi/2*sin(pi*patches.x);
end%if
```

Simulate Set the initial conditions of a simulation to be zero. Mark that edge of patches are not to be used in the projective extrapolation by setting initial values to NaN.

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

Set the desired macro- and microscale time-steps over the time domain. The macroscale step is in proportion to the effective mean diffusion time on the macroscale, here $1/(A_0\pi^2) \approx 1$ so for macro-scale error less than 1% need $\Delta t < 0.24$, so use 0.1 say.

The burst time depends upon the sub-patch effective diffusion rate β where here rate $\beta \approx \pi^2 A_0/h^2 \approx 2000$ for patch width $h \approx 0.02$: use the formula from the Manual, with some extra factor, and rounded to the nearest multiple of the time micro-periodicity.

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

Time the projective integration simulation.

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

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

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

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

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

```
xs([1 end],:) = nan;
for k = 1:2, subplot(2,2,2+k)
  surf(tss,xs(:),uss',  'EdgeColor','none')
  ylabel('space $x$'), xlabel('time $t$'), zlabel('$u(x,t)$')
  colormap(0.7*hsv), axis tight, view(62-4*k,45)
end
ifOurCf2eps(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).

```
function [ts, ucts] = heteroBurstF(ti, ui, bT)
  global microTimePeriod
  [ts,ucts] = ode45( @patchSys1,ti+(0:microTimePeriod:bT),ui(:));
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

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

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]

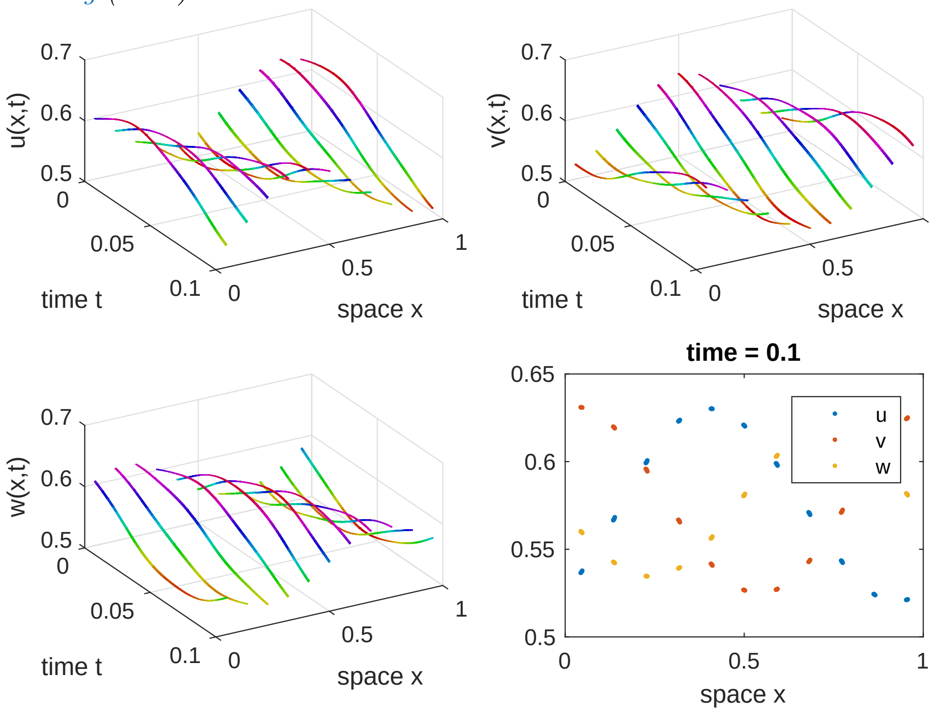
```
global alpha ex5p1
ex5p1 = 0; % set to 1 for L&O example of p.27
alpha = 0.001 % phenomenological damping parameter
```

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).*




```
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.

```
dx = 1/2000 %1/6000 %p.27
mPeriod = round(epsilon/dx)
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).

```
global patches
nPatch = 11 %24 %p.6, odd is slightly cleaner
nSubP = mPeriod+2
ratio = nPatch*epsilon
configPatches1(@heteroLanLif1D,[0 1],nan,nPatch ...
    ,0,ratio,nSubP,'EdgyInt',true ...
    ,'hetCoeffs',a);
assert(abs(dx-diff(patches.x(2:3)))<1e-10 ...
      ,'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 $|\vec{M}(x,0)| = 1$.

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

Integrate using standard integrators.

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

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

```
xs = squeeze(patches.x);
Ms = reshape(Ms,length(ts),nSubP,3,nPatch);
Ms(:,[1 end],:,:) = nan; % nan patch edges
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}.

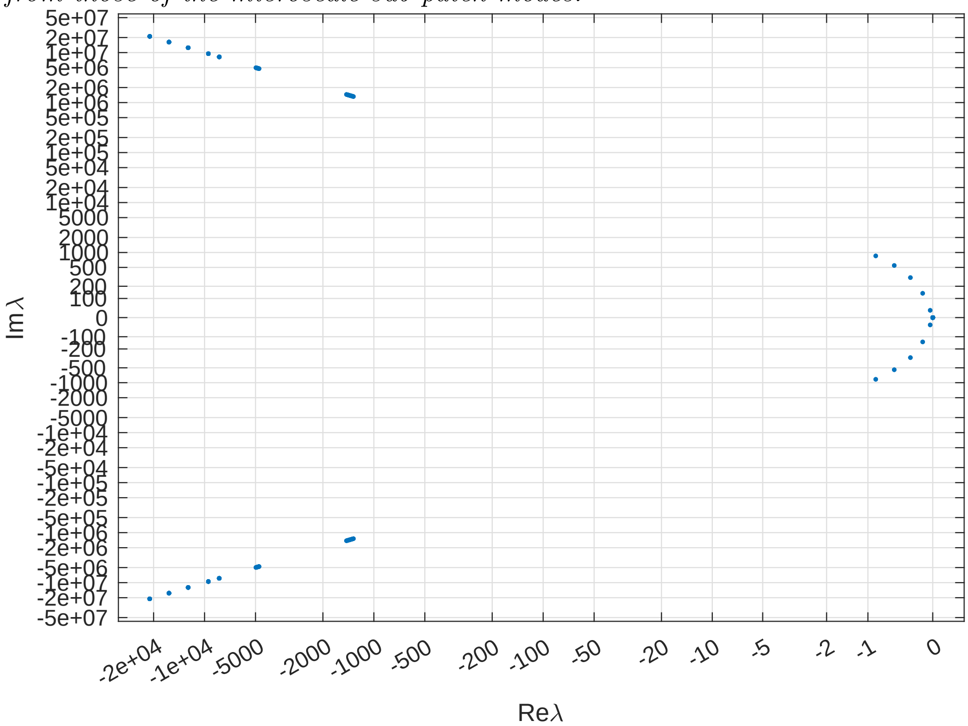
```
Mabs = sqrt( sum(Ms.^2,3) );
meanMabs = mean(Mabs(:),'omitnan')
stdevMabs = std(Mabs(:),'omitnan')
```

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

```
global OurCf2eps
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.*




```
figure(1),clf
if length(ts)>50
  [~,j]=min(abs(ts(:)-linspace(ts(1),ts(end),50)));
  else j=1:length(ts); end
uvw='uvw';
for p=1:3
  subplot(2,2,p)
  mesh(ts(j),xs(:),Ms(:,j,p))
  view(60,40), colormap(0.8*hsv)
  xlabel('time $t$'), ylabel('space $x$')
  zlabel(['$' uvw(p) '(x,t)$'])
end
```

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

```
subplot(2,2,4)
plot(xs(:),squeeze(Ms(:,end,:)),'.')
xlabel('space $x$'), legend(uvw(1),uvw(2),uvw(3))
title(['time = ' num2str(ts(end),4)])
ifOurCf2eps([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 $N = \texttt{nPatch}$ and $n = \texttt{nSubP} - 2$, 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.

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

Form the Jacobian by numerical differentiation.

```
delta=1e-7;
nJac=length(i);
Jac=nan(nJac);
for j=1:nJac
  M=Me; M(i(j))=M(i(j))+delta;
  fj=patchSys1(0,M(:));
  Jac(:,j)=(fj(i)-f0(i))/delta;
end
```

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

```
eval = eig(Jac);
[~,k] = sort(abs(eval));
eval = eval(k);
nZero = sum(abs(eval)<1)
nCent = sum(abs(real(eval))<1e5*alpha)
nSlow = sum(abs(eval)<1e5)
```

Plot the spectrum of eigenvalues on quasi-log axes.

```
figure(2),clf
plot(real(eval),imag(eval),'.');
xlabel('$\Re\lambda$'), ylabel('$\Im\lambda$')
quasiLogAxes(1,100);
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).

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

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

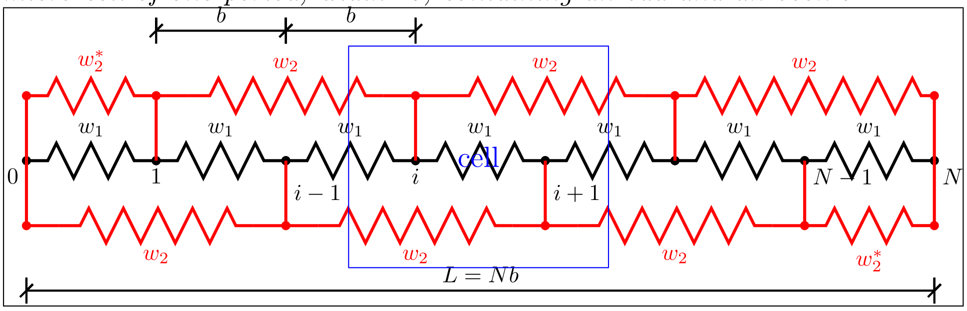
```
  a = patches.cs ...
     +ex5p1*(0.1+0.25*sin(2*pi*(patches.x(2:end,:,:,:)-dx/2)+1.1));
  H = diff(a.*diff(M))/dx^2;
```

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)):

```
  i = 2:size(M,1)-1;   % interior points in a patch
  MH=nan+H; % preallocate for MxH
  MH(:,3,:,:) = M(i,1,:,:).*H(:,2,:,:)-M(i,2,:,:).*H(:,1,:,:);
  MH(:,2,:,:) = M(i,3,:,:).*H(:,1,:,:)-M(i,1,:,:).*H(:,3,:,:);
  MH(:,1,:,:) = M(i,2,:,:).*H(:,3,:,:)-M(i,3,:,:).*H(:,2,:,:);
  MMH=nan+H; % preallocate for MxMxH
  MMH(:,3,:,:)= M(i,1,:,:).*MH(:,2,:,:)-M(i,2,:,:).*MH(:,1,:,:);
  MMH(:,2,:,:)= M(i,3,:,:).*MH(:,1,:,:)-M(i,1,:,:).*MH(:,3,:,:);
  MMH(:,1,:,:)= M(i,2,:,:).*MH(:,3,:,:)-M(i,3,:,:).*MH(:,2,:,:);
  Mt = nan+M; % preallocate output array
  Mt(i,:,:,:) = -MH-alpha*MMH;
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,

$$\begin{aligned} \epsilon_i^p &:= \frac{1}{pb}(u_{i+p/2} - u_{i-p/2}), & \sigma_i^p &:= w_p'(\epsilon_i^p), \\ \frac{\partial^2 u_i}{\partial t^2} &= \sum_{p=1}^{2} \frac{1}{pb}(\sigma_{i+p/2}^p - \sigma_{i-p/2}^p), & w_p'(\epsilon) &:= \epsilon - M_p\epsilon^3 + \epsilon^5. \end{aligned} \tag{3.9}$$

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

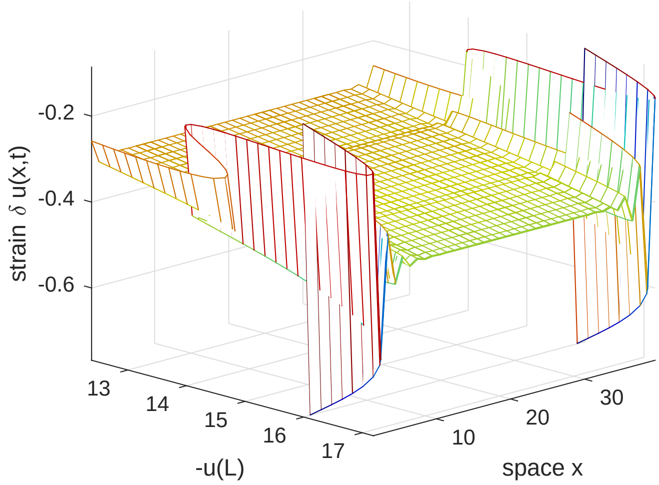


Figure 3.24: the case of microscale 'instability' appears as fluctuations close to both boundaries. As the system is physically compressed, the equilibrium curve has complicated folds, as shown here (and Figure 3.27(b)).

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.

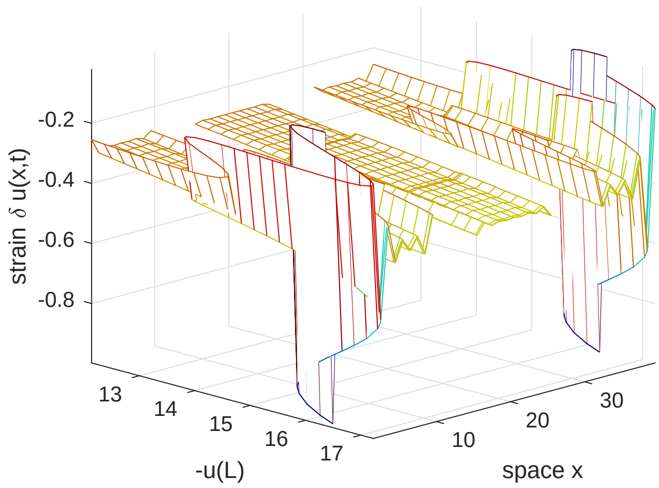
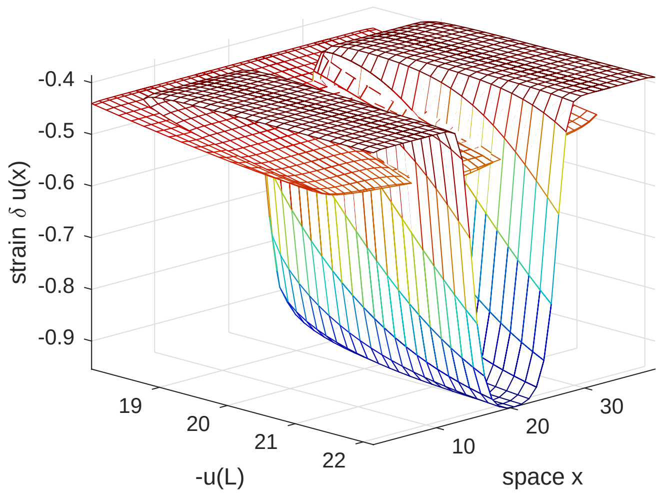


Figure 3.26: the case of large scale 'instability'. Spatial structure appears in the middle of the domain. As the system is physically compressed, the equilibrium curve has complicated folds, as shown here and in Figure 3.27(a).



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,

Table 3.5: Interesting equilibria for the cases of large scale instability: $M_1 := -1$, $M_2 := 3$ (Figures 3.26 and 3.27(a)).

$-u(L)$	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 the physical displacements form the array

$$\mathtt{u} = \begin{bmatrix} u_1 & u_2 \\ u_3 & u_4 \\ u_5 & u_6 \\ \vdots & \vdots \end{bmatrix}.$$

Then corresponding velocities are adjoined as 3rd and 4th column.

```
clear all
global b M vis
b = 1   % separation of lattice points
N = 42  % # lattice steps in L
L = b*N % length of domain
```

The nonlinear coefficients of stress-strain are in array `M`, chosen by `theCase`.

```
theCase = 2
switch theCase
case 1, M = [0 0 0 0]  % linear spring coefficients
case 2, M = [ 2 1 1 1] % micro scale instability??
case 3, M = [-1 3 1 1] % large scale instability??
end% switch
vis = 0.1 % does not appear to affect the equilibria
tEnd = 25
```

Patch parameters: here `nSubP` is the number of cells.

```
edgyInt = true
nSubP = 6, nPatch = 5 % gives full-domain on N=42, dx=2
%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.

```
global patches
configPatches1(@heteroNLE,[0 L],'equispace',nPatch ...
```

```
    ,0,2*b,nSubP,'EdgyInt',edgyInt);
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.

```
u0 = [ sin(pi/L*xx)  -0*0.14*cos(pi/L*xx) ];
tic
[ts,ust] = ode23(@patchSys1, tEnd*linspace(0,1,41), u0(:) ...
               ,[],patches,0);
cpuIntegrateTime = toc
```

Plot space-time surface of the simulation To see the edge values of the patches, interpolate and then adjoin a row of `nan`s 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.

```
xs = reshape( permute( xx ,[2 1 3 4]), 2*nSubP,nPatch);
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.

```
uvs = reshape( permute( reshape(ust ...
      ,length(ts),nSubP,4,1,nPatch) ,[2 3 1 4 5]) ,nSubP,[],1,nPatch);
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.

```
us = reshape( permute( uvs(:,1:2,:,:) ...
     ,[2 1 4 3]) ,2*nSubP,nPatch,[]);
us(end+1,:,:) = nan;
us = reshape(us,[],length(ts));
```

Plot space-time surface of displacements over the macroscale duration of the simulation.

```
  figure(1), clf()
  mesh(ts,xs(:),us)
  view(60,40), colormap(0.8*jet), axis tight
  xlabel('time $t$'), ylabel('space $x$'), zlabel('$u(x,t)$')
```

Ditto for the velocity.

```
vs = reshape( permute( uvs(:,3:4,:,:) ...
     ,[2 1 4 3]) ,2*nSubP,nPatch,[]);
vs(end+1,:,:) = nan;
vs = reshape(vs,[],length(ts));
  figure(2), clf()
```

```
  mesh(ts,xs(:),vs)
  view(60,40), colormap(0.8*jet), axis tight
  xlabel('time $t$'), ylabel('space $x$'), zlabel('$v(x,t)$')
  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.

```
muL0 = 12+6*(theCase==3)
u0 = [ -muL0*xx/L 0*xx ];
u0([1 end],:,:,:)=nan;
patches.i = find(~isnan(u0));
nVars=length(patches.i)
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.

```
disp('Searching for equilibria, may take 1000+ secs')
[uv0,vec0]=init_EP_EP(@matContSys,ueq,muL0,[1]);
opt=contset; % initialise MatCont options
opt=contset(opt,'Singularities',true); %to report branch points, p.24
opt=contset(opt,'MaxNumPoints',400); % restricts how far matcont goes
opt=contset(opt,'Backward',true); % strangely, needs to go backwards??
[uv,vec,s,h,f]=cont(@equilibrium, uv0, [], opt); %MatCont continuation
```

Post-process the report

```
disp('List of interesting critical points')
muLs=uv(nVars+1,:);
for j=1:numel(s)
   disp([num2str(muLs(s(j).index),5) ' & ' s(j).msg ' \\'])
end
```

Find a range of parameter and corresponding indices where all the critical points occur.

```
p1=muLs(end); pe=muLs(1);
if numel(s)>3, for j=2:numel(s)-1
    p1=min(p1,muLs(s(j).index));
    pe=max(pe,muLs(s(j).index));
end, end
pMid=(p1+pe)/2, pWid=abs(pe-p1)
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.

```
nPars=numel(iPars)
dP=ceil((nPars-1)/60)
```

```
iP=1:dP:nPars;
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.

```
uvs=nan(numel(iP),numel(u0));
uvs(:,patches.i)=uv(1:nVars,iPars(iP))';
uvs = reshape( permute( reshape(uvs ...
      ,length(muLP),nSubP,4,1,nPatch) ,[2 3 1 4 5]) ,nSubP,[],1,nPatch);
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.

```
us = reshape( permute( uvs(:,1:2,:,:) ...
     ,[2 1 4 3]) ,2*nSubP,nPatch,[]);
us(end+1,:,:) = nan;
us = reshape(us,[],length(muLP));
```

Plot space-time surface of displacements over the macroscale duration of the simulation.

```
  figure(4), clf()
  mesh(muLP,xs(:),us)
  view(60,40), colormap(0.8*jet), axis tight
  xlabel('-u(L)'), ylabel('space $x$'), zlabel('$u(x)$')
```

Plot space-time surface of strain, differences in displacements, over the parameter variation.

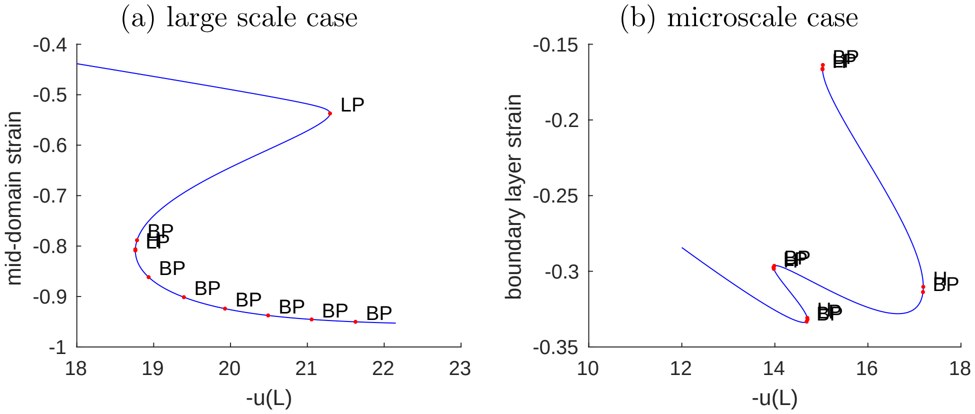
```
  figure(5), clf()
  mesh(muLP,xs(1:end-1),diff(us))
  view(45,20), colormap(0.8*jet), axis tight
  xlabel('$-u(L)$'), ylabel('space $x$'), zlabel('strain $\delta u(x)$')
  ifOurCf2eps(['Comb22diffu' num2str(theCase)],[12 9])%optionally save
```

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??).

```
uvs = nan(numel(muLs),numel(u0));
uvs(:,patches.i) = uv(1:nVars,:)';
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.




```
if theCase==2, thePatch=1;
else thePatch=(nPatch+1)/2;
end%if
  figure(7),clf
  du = diff( uvs(:,nSubP/2,1:2,thePatch) ,1,3);
  cpl([muLs;du'],[],s);
  xlabel('$-u(L)$')
  if thePatch==1,  ylabel('boundary layer strain')
  else ylabel('mid-domain strain')
  end
  ifOurCf2eps(['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.

```
function out = matContSys%(t,coordinates,flag,y,z)
out{1} = [];%@init;
out{2} = @dudtSys;
out{3} = [];%@jacobian;
out{4} = [];%@jacobianp;
out{5} = [];%@hessians;
out{6} = [];%@hessiansp;
out{7} = [];
out{8} = [];
out{9} = [];
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`.

```
function ut = dudtSys(t,u,p)
global patches
```

The 4 here is the number of variables in each micro-cell, that is, notionally 'at' each x-grid point.

```
U=nan(1,4)+patches.x;
U(patches.i)=u(:);
Ut=patchSys1(t,U,patches,p);
ut=Ut(patches.i);
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`.

```
function uvt = heteroNLE(t,uv,patches,muL)
  if nargin<4, muL=0; end% default end displacement is zero
  global b M vis
```

Separate state vector into displacement and velocity fields: u_{ijI} is the displacement at the jth point in the ith 2-cell in the Ith patch; similarly for velocity v_{ijI}. That is, physically neighbouring points have different j, whereas physical next-to-neighbours have i different by one.

```
  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.

```
u(1,:,:,1)=0;
v(1,:,:,1)=0;
u(end,:,:,end)=-muL;
v(end,:,:,end)=0;
```

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

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

Set corresponding nonlinear stresses

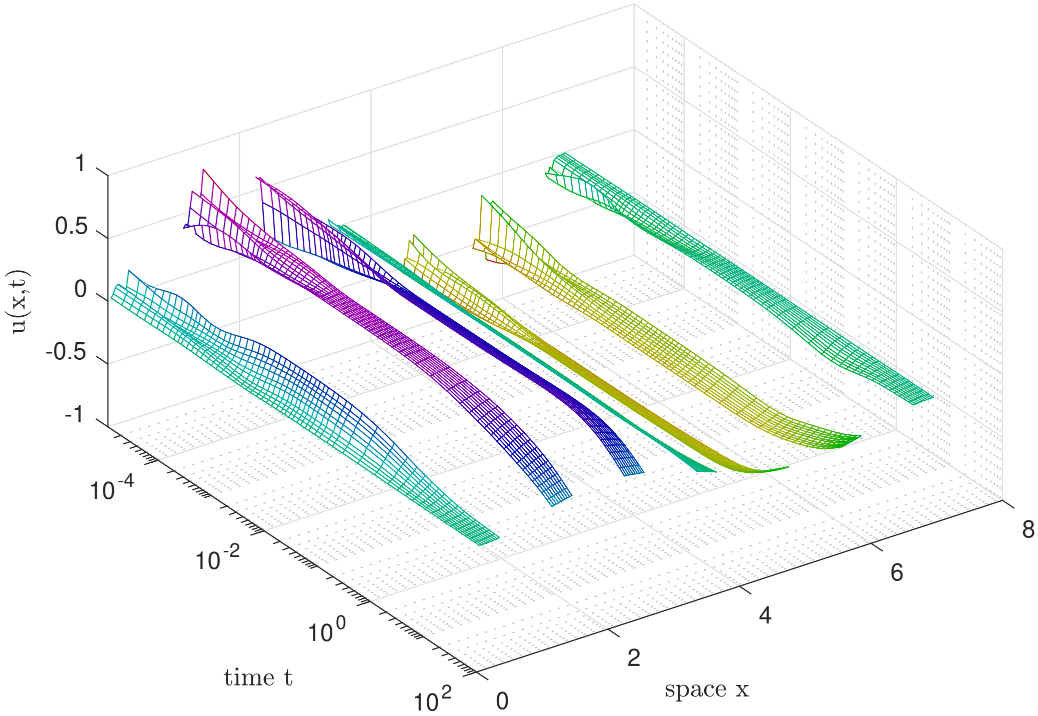
```
  sig2 = eps2-M(2)*eps2.^3+M(4)*eps2.^5;
  sig1 = eps1-M(1)*eps1.^3+M(3)*eps1.^5;
```

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

```
  uvt = nan+uv;          % preallocate output array
  i=2:size(uv,1)-1;
  % rate of change of position
  uvt(i,1:2,:,:) = v(i,:,:,:);
  % rate of change of velocity +some artificial viscosity??
  uvt(i,3:4,:,:) = diff(sig2) ...
    +[ sig1(i,1,:,:)-sig1(i-1,2,:,:)  diff(sig1(i,:,:,:),1,2)] ...
  +vis*[ vx1(i,1,:,:)-vx1(i-1,2,:,:)  diff(vx1(i,:,:,:),1,2) ];

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

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

$$u_t = -D[c_1(x)Du] \quad \text{where operator } D := \partial_x(c_2(x)\partial_x), \tag{3.10}$$

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

$$\dot{u}_i = -D[c_{i1} D u_i] \quad \text{where operator } D := \delta(c_{i2}\delta)/dx^2$$

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).

```
clear all
basename = mfilename
%global OurCf2eps, OurCf2eps=true %optional to save plots
nGap = 3 % controls size of gap between patches
nPtsPeriod = 5
dx = 0.5/nGap/nPtsPeriod
```

Create some random heterogeneous coefficients, log-uniform.

```
csVar = 1
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` $= 0$.

```
nPatch = 7
nSubP = 2*nPtsPeriod+4 % or +2 for not-edgyInt
Len = nPatch;
ordCC = 0;
dom.type = 'equispace';
dom.bcOffset = 0.5 % for BC type
patches = configPatches1(@hyperDiffPDE,[0 Len],dom ...
    ,nPatch,ordCC,dx,nSubP,'EdgyInt',true,'nEdge',2 ...
    ,'hetCoeffs',cs);
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.

```
u0 = sin(2*pi/Len*patches.x).*rand(nSubP,1,1,nPatch);
tic
[ts,us] = ode15s(@patchSys1, [0 100], u0(:) ,[],patches);
simulateTime = toc
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.

```
figure(1),clf
xs([1:2 end-1:end],:) = nan;
t0=min(find(ts>1e-5));
mesh(ts(t0:3:end),xs(:),us(t0:3:end,:)'),  view(55,50)
```

```
colormap(0.7*hsv)
xlabel('time $t$'), ylabel('space $x$'), zlabel('$u(x,t)$')
ca=gca;  ca.XScale='log';  ca.XLim=ts([t0 end]);
ifOurCf2eps([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 $D = \partial_x(c_2(x)\partial_x)$.

```
function ut=hyperDiffPDE(t,u,patches)
  dx=diff(patches.x(1:2));  % microscale spacing
```

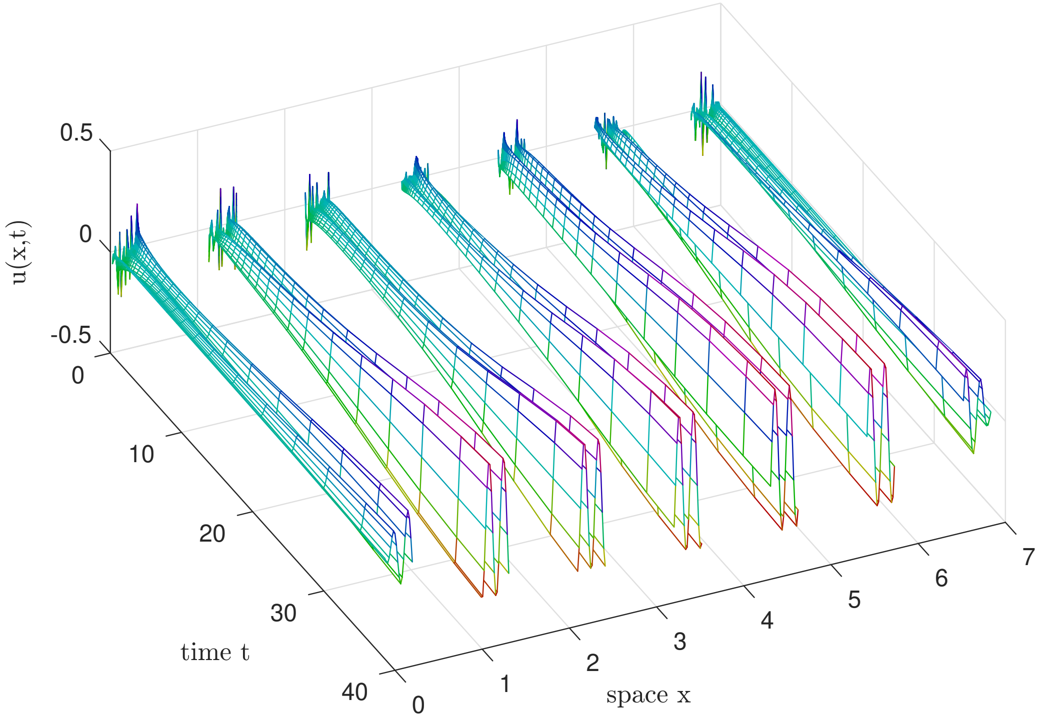
Code Dirichlet boundary conditions of zero function and derivative at left-end of left-patch, and right-end of right-patch. For slightly simpler coding, squeeze out the two singleton dimensions.

```
  u = squeeze(u);
  if ~patches.periodic % discretise BC u=u_x=0
      u(1:2,1)=0;
      u(end-1:end,end)=0;
  end%if
```

Here code straightforward centred discretisation in space.

```
  ut = nan+u;   % preallocate output array
  v = patches.cs(2:end,1).*diff(patches.cs(:,2).*diff(u))/dx^2;
  ut(3:end-2,:) = -diff(patches.cs(2:end-1,2).*diff(v))/dx^2 ;
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

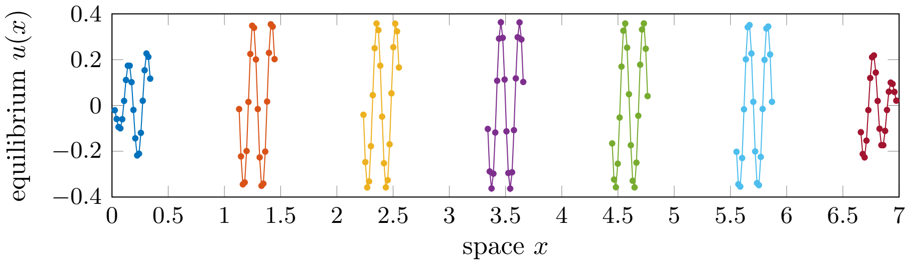
Section contents

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

$$\partial_t u = -(1 + \partial_x^2/k_0^2)^2 u + \mathrm{Ra}\, u - u^3, \tag{3.11}$$

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.

```
clear all, close all
%global OurCf2eps, OurCf2eps=true %optional to save plots
Ra = 0.1 % Ra>0 leads to patterns
nGap = 3
%waveLength = 0.496688741721854 /nGap %for nPatch==5
waveLength = 0.497630331753555 /nGap %for nPatch==7
%waveLength = 0.5 /nGap %for periodic case
nPtsPeriod = 10
dx = waveLength/nPtsPeriod
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 `ordCC` $= 4$ provides values for the inter-patch coupling conditions.

```
nPatch = 7
nSubP = 2*nPtsPeriod+4
%nSubP = 2*nGap*nPtsPeriod+4 % full-domain
Len = nPatch;
ordCC = 4;
dom.type='equispace';
dom.bcOffset=0.5
patches = configPatches1(@SwiftHohenbergPDE,[0 Len],dom ...
    ,nPatch,ordCC,dx,nSubP,'EdgyInt',true,'nEdge',2);
xs=squeeze(patches.x);
```

3.17.0.1 Find equilibrium with fsolve

Start the search from some guess.

```
fprintf('\n**** Find equilibrium with fsolve\n')
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.

```
u([1:2 end-1:end],:) = nan;
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).

```
tic
[u(patches.i),res] = fsolve(@(v) theRes(v,patches,k0,Ra) ...
    ,u(patches.i) ,optimoptions('fsolve','Display','off'));
solveTime = toc
normRes = norm(res)
assert(normRes<1e-6,'**** fsolve solution not accurate')
```

Plot the equilibrium see Figure 3.30.

```
figure(1),clf
subplot(2,1,1)
plot(xs,squeeze(u),'.-')
xlabel('space $x$'),ylabel('equilibrium $u(x)$')
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.

```
fprintf('\n**** Simulate in time\n')
u0 = 0*patches.x+0.1*randn(nSubP,1,1,nPatch);
tic
[ts,us] = ode15s(@patchSys1, [0 40], u0(:) ,[],patches,k0,Ra);
simulateTime = toc
us = reshape(us,length(ts),numel(patches.x(:)),[]);
```

Plot the simulation in Figure 3.29.

```
figure(2),clf
xs([1:2 end-1:end],:) = nan;
mesh(ts(1:3:end),xs(:),us(1:3:end,:)'),  view(65,60)
colormap(0.7*hsv)
xlabel('time $t$'), ylabel('space $x$'), zlabel('$u(x,t)$')
ifOurCf2eps([mfilename 'Uxt'])
```

Fin.

3.17.1 The Swift–Hohenberg PDE and BCs inside patches

As a microscale discretisation of Swift–Hohenberg PDE $u_t = -(1+\partial_x^2/k_0^2)^2u + \mathrm{Ra}\,u - u^3$, here code straightforward centred discretisation in space.

```
function ut=SwiftHohenbergPDE(t,u,patches,k0,Ra)
  dx=diff(patches.x(1:2));  % microscale spacing
  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.

```
  u = squeeze(u);
  u(1:2,1)=0;
  u(end-1:end,end)=0;
```

Here code straightforward centred discretisation in space.

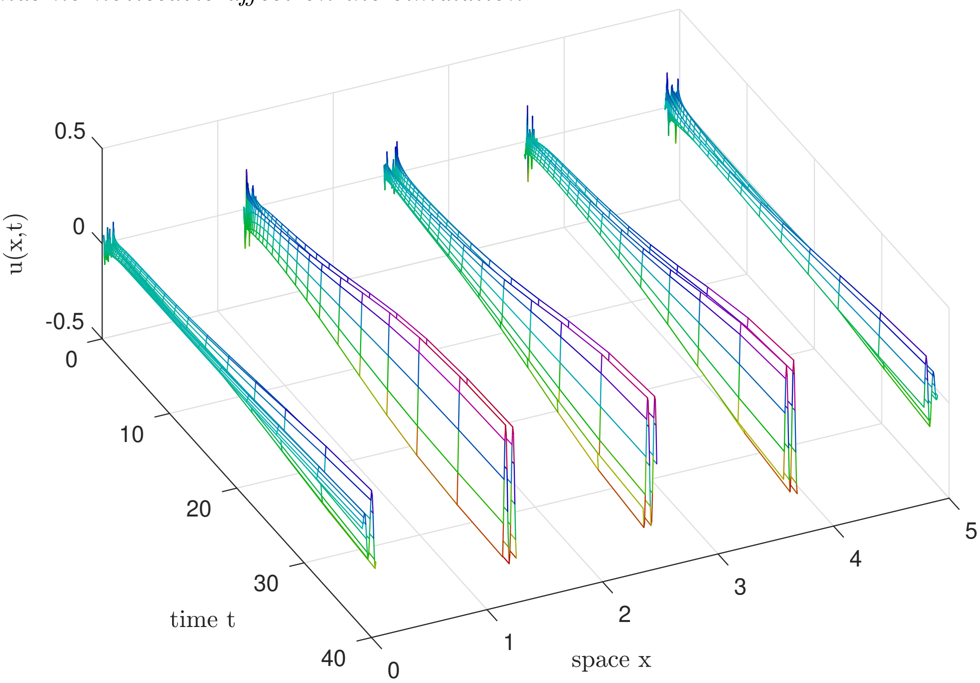
```
  ut=nan+u;          % preallocate output array
  v = u(2:end-1,:)+diff(u,2)/dx^2/k0^2;
  ut(i,:) = -( v(2:end-1,:)+diff(v,2)/dx^2/k0^2 ) ...
    +Ra*u(i,:) -u(i,:).^3;
end
```

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.

```
function f=theRes(u,patches,k0,Ra)
  v=nan(size(patches.x));
  v(patches.i) = u;
  f = patchSys1(0,v(:),patches,k0,Ra);
  f = f(patches.i);
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

Section contents

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

$$\partial_t u = -D[c_1(x)Du] + \mathrm{Ra}\, u - u^3, \quad D := 1 + \partial_x[c_2(x)\partial_x \cdot]/k_0^2, \tag{3.12}$$

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 $k_0 \approx 101$.

```
clear all
%global OurCf2eps, OurCf2eps=true %optional to save plots
basename = ['r' num2str(floor(1e5*rem(now,1))) mfilename]
Ra = 0.1  % Ra>0 leads to patterns
nGap = 8 % controls size of gap between patches
```

```
waveLength = 0.496688741721854 /nGap %for nPatch==5
%waveLength = 0.497630331753555 /nGap %for nPatch==7
%waveLength = 0.5 /nGap %for periodic case
nPtsPeriod = 10
dx = waveLength/nPtsPeriod
k0 = 2*pi/waveLength
```

Create some random heterogeneous coefficients.

```
heteroVar = 0.99*[1 1] % must be <2
cl = 1./(1-heteroVar/2+heteroVar.*rand(nPtsPeriod,2));
cRange = quantile(cl,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` $= 0$.

```
nPatch = 5
nSubP = 2*nPtsPeriod+4 % +2 for not-edgyInt
%nSubP = 2*nGap*nPtsPeriod+4 % approx full-domain
Len = nPatch;
ordCC = 0;
dom.type='equispace';
dom.bcOffset=0.5
patches = configPatches1(@heteroSwiftHohenbergPDE,[0 Len],dom ...
    ,nPatch,ordCC,dx,nSubP,'EdgyInt',true,'nEdge',2 ...
    ,'hetCoeffs',cl);
xs=squeeze(patches.x);
```

3.18.0.1 Explore the Jacobian

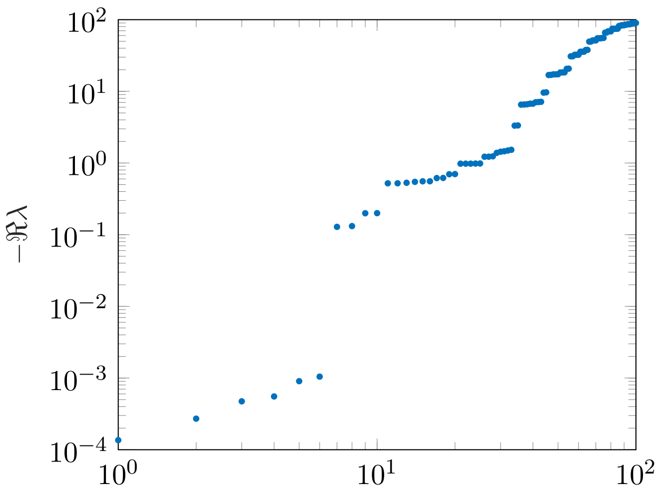
Finds that with periodic patches, everything is symmetric. However, for equispace or chebyshev, the patch coupling is not symmetric—is this to be expected?

```
fprintf('\n**** Explore the Jacobian\n')
u0 = 0*patches.x;
u0([1:2 end-1:end],:) = nan;
patches.i = find(~isnan(u0));
nVars = numel(patches.i)
Jac = nan(nVars);
for j=1:nVars
    Jac(:,j)=theRes((1:nVars)==j,patches,k0,0,0);
end
```

Check on the symmetry of the Jacobian

```
nonSymmetric = norm(Jac-Jac')
Jac(abs(Jac)<1e-12)=0;
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.




```
antiJac(abs(antiJac)<1e-12)=0;
figure(6),clf
spy(Jac,'.'),hold on, spy(antiJac,'rx'),hold off
if nonSymmetric>5e-9, warning('failed symmetry'),
else Jac = (Jac+Jac')/2; %tweak to symmetry
end
```

Compute eigenvalues and eigenvectors.

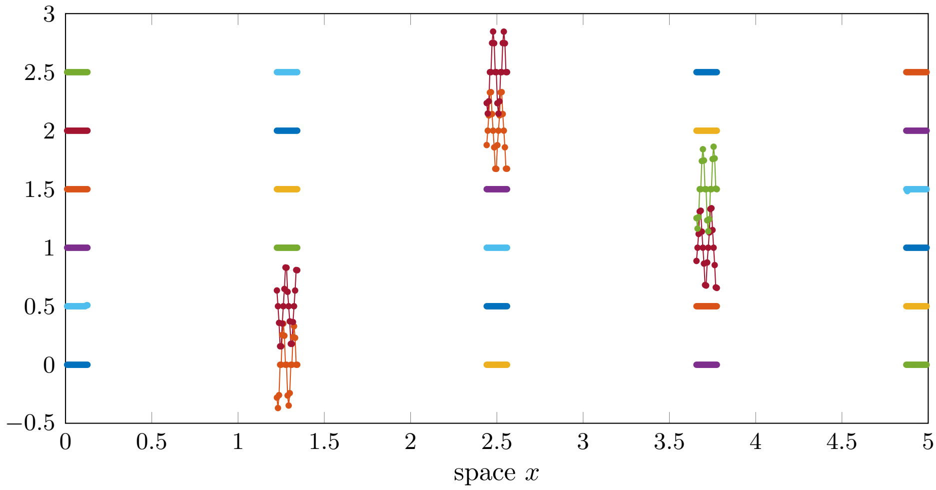
```
figure(5),clf
[evec,mEval] = eig(-Jac ,'vector');
[~,j]=sort(real(mEval));
mEval=mEval(j); evec=evec(:,j);
loglog(real(mEval),'.')
ylabel('$-\Re\lambda$')
ifOurCf2tex([basename 'Eval'])%optionally save
```

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.

```
logGaps=diff(log10(real(mEval)));
[~,j]=sort(-logGaps);
%someLogGaps=[logGaps(j(1:5)) j(1:5)]
if logGaps(j(2))<0.4*logGaps(j(1)), nSlow=j(1)
else nSlow=min( sort(j(1:2)) , 3*nPatch)
end
log10Gap=logGaps(nSlow)
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.

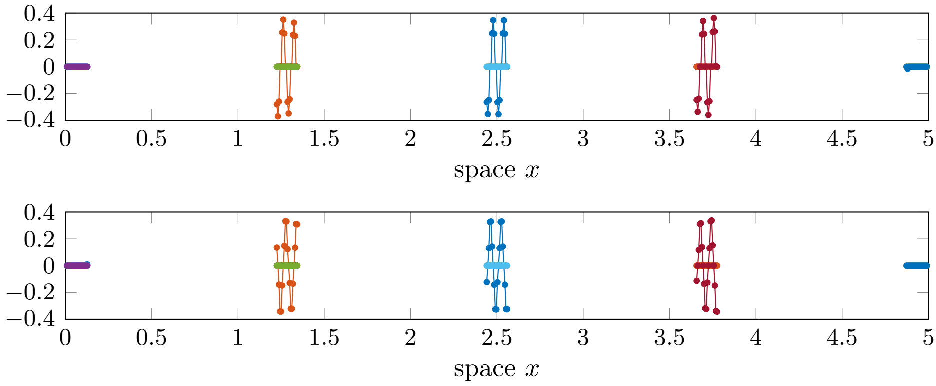



```
js=find(imag(mEval)>0);
evec(:,js)=imag(evec(:,js));
evec=real(evec);
if numel(nSlow)==1, S = spcart(evec(:,1:nSlow));
else  S = spcart(evec(:,1:nSlow(1)));
   S = [S spcart(evec(:,nSlow(1)+1:nSlow(2))) ];
end;
figure(3),clf
vStep=ceil(max(abs(S(:)))*10+1)/10
for j=1:nSlow(end)
  u0(patches.i)=S(:,j);
  plot(xs,vStep*(j-1)+squeeze(u0),'.-'),hold on
end
hold off, xlabel('space $x$')
ifOurCf2tex([basename 'Evec'])%optionally save
```

Reorganise the eigenvectors to maybe clarify.

```
[i,j]=find(abs(S)>vStep/2);
j=find([1;diff(j)]);
[i,k]=sort(i(j));
figure(4)
for p=1:2
  clf,subplot(2,1,1)
  for j=p:2:numel(k)
    u0(patches.i)=S(:,k(j));
    plot(xs,squeeze(u0),'.-'),hold on
  end% for j
  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.




```
  ifOurCf2tex([basename 'Evec' num2str(p)])%optionally save
end%for p
```

3.18.0.2 Find an equilibrium with fsolve

Start the search from some guess.

```
fprintf('\n**** Find equilibrium with fsolve\n')
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.

```
u([1:2 end-1:end],:) = nan;
patches.i = find(~isnan(u));
```

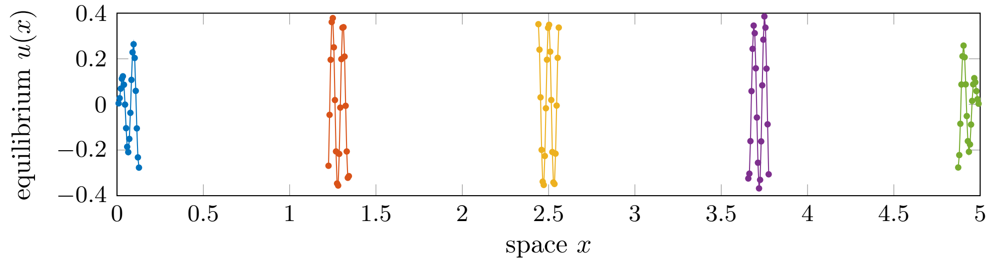
Seek the equilibrium, and report the norm of the residual, via the generic patch system wrapper `theRes` (Section 3.18.2).

```
tic
[u(patches.i),res] = fsolve(@(v) theRes(v,patches,k0,Ra,1) ...
    ,u(patches.i) ,optimoptions('fsolve','Display','off'));
solveTime = toc
normRes = norm(res)
if normRes>1e-7, warning('residual large: bad equilibrium'),end
```

Plot the equilibrium see Figure 3.35.

```
figure(1),clf
subplot(2,1,1)
plot(xs,squeeze(u),'.-')
xlabel('space $x$'),ylabel('equilibrium $u(x)$')
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.

```
fprintf('\n**** Simulate in time\n')
u0 = 0*sin(2*pi/waveLength*patches.x)+0.1*randn(nSubP,1,1,nPatch);
tic
[ts,us] = ode15s(@patchSys1, [0 40], u0(:) ,[],patches,k0,Ra,1);
simulateTime = toc
us = reshape(us,length(ts),numel(patches.x(:)),[]);
```

Plot the simulation in Figure 3.31.

```
figure(2),clf
xs([1:2 end-1:end],:) = nan;
mesh(ts(1:3:end),xs(:),us(1:3:end,:)'),  view(65,60)
colormap(0.7*hsv)
xlabel('time $t$'), ylabel('space $x$'), zlabel('$u(x,t)$')
ifOurCf2eps([basename 'Uxt'])
```

Fin.

3.18.1 Heterogeneous SwiftHohenberg PDE+BCs inside patches

As a microscale discretisation of Swift–Hohenberg PDE $u_t = -D[c_1(x)Du] + \mathrm{Ra}\,u - u^3$, where heterogeneous operator $D = 1 + \partial_x(c_2(x)\partial_x)/k_0^2$.

```
function ut=heteroSwiftHohenbergPDE(t,u,patches,k0,Ra,cubic)
  dx=diff(patches.x(1:2));  % microscale spacing
  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.

```
  u = squeeze(u);
  if ~patches.periodic
    switch 1
```

```
    case 1 % these are u=u_x=0
      u(1:2,1)=0;
      u(end-1:end,end)=0;
    case 2 % these are u=u_{xx}=0
      u(1:2,1) = [-u(3,1); 0];
      u(end-1:end,end) = [0; -u(end-2,end)];
    end% case
  end%if
```

Here code straightforward centred discretisation in space.

```
  ut = nan+u;         % preallocate output array
  v = u(2:end-1,:)+diff(patches.cs(:      ,2).*diff(u))/dx^2/k0^2;
  v = v.*patches.cs(2:end,1);
  v = v(2:end-1,:)+diff(patches.cs(2:end-1,2).*diff(v))/dx^2/k0^2;
  ut(i,:) = -v +Ra*u(i,:) -cubic*u(i,:).^3;
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.

```
function f=theRes(u,patches,k0,Ra,cubic)
  v=nan(size(patches.x));
  v(patches.i) = u;
  f = patchSys1(0,v(:),patches,k0,Ra,cubic);
  f = f(patches.i);
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.

```
function f=theRes(u)
  global patches
  switch numel(size(patches.x))
    case 4, pSys = @patchSys1;
            v=nan(size(patches.x));
    case 5, pSys = @patchSys2;
            v=nan(size(patches.x+patches.y));
    case 6, pSys = @patchSys3;
            v=nan(size(patches.x+patches.y+patches.z));
    otherwise error('number of dimensions is somehow wrong')
  end%switch
  v(patches.i) = u;
  f = pSys(1,v(:),patches);
  f = f(patches.i);
end%function theRes
```

3.20 `quasiLogAxes()`: transforms current axes of plot(s) to quasi-log

This function transforms the plots in the current axes. It rescales specified coordinates and labels the axes and its 2D or 3D plot(s). 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. This nonlinear rescaling is useful in other scenarios also.

```
function quasiLogAxes(xScale,yScale,zScale,cScale)
```

Input This function rescales the *current axes* (you may need to invoke `set()` to change to the axes you require). It rescales the existing plots (do not do further plots into the same axes).

- `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 plot and its transformation.

```
if nargin==0
   % generate some data
   n=99;  fast=(rand(n,1)<0.8);
   z = -rand(n,1).*(1+1e3*fast)+1i*randn(n,1).*(5+1e2*fast);
   % plot data and transform axes
   plot(real(z),imag(z),'.');
   xlabel('real-part'), ylabel('imag-part')
   title('un-transformed plot, pausing for 3 secs'), pause(3)
   quasiLogAxes(1,10);
   title('transformed plot')
   return
end% example
```

Default values for scaling, `inf` denotes no transformation of that axis.

```
if nargin<4, cScale=inf; end
if nargin<3, zScale=inf; end
if nargin<2, yScale=inf; end
if nargin<1, xScale=inf; end
assert(class(xScale)=="double" ...
      ,"May 2023 version of quasiLogAxes does not accept a handle")
```

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.

```
xlim0=xlim; ylim0=ylim; zlim0=zlim; clim0=caxis;
theAxes = gca;  %get(handle(1),'parent');
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.

```
xFac=1e-99; yFac=xFac; zFac=xFac; cFac=xFac;
for kk=1:numel(theAxes.Children)
  handle = theAxes.Children(kk);
  for k=1:length(handle)
    if ~isinf(xScale)
    temp = asinh(handle(k).XData/xScale);
    xFac = max(xFac, max(abs(temp(:)),[],'omitnan') );
    end
    if ~isinf(yScale)
    temp = asinh(handle(k).YData/yScale);
    yFac = max(yFac, max(abs(temp(:)),[],'omitnan') );
    end
    if ~isinf(zScale)
    temp = asinh(handle(k).ZData/zScale);
    zFac = max(zFac, max(abs(temp(:)),[],'omitnan') );
    end
    if ~isinf(cScale)
    temp = asinh(handle(k).CData/cScale);
    cFac = max(cFac, max(abs(temp(:)),[],'omitnan') );
    end
  end%for k
end%for kk
xFac=9/xFac; yFac=9/yFac; zFac=9/zFac; cFac=9/cFac;
```

Scale all the plot data in the axes. 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.

```
xlim1=[Inf -Inf]; ylim1=xlim1; zlim1=xlim1; clim1=xlim1;
for kk=1:numel(theAxes.Children)
  handle = theAxes.Children(kk);
  for k=1:length(handle)
    assert(~strcmp(handle(k).UserData,'quasiLogAxes'), ...
       'Replot graph---it appears plot data is already transformed')
```

```
    if ~isinf(cScale)
    handle(k).CData = cFac*asinh(handle(k).CData/cScale);
    climk=[min(handle(k).CData(:)) max(handle(k).CData(:))];
    clim1=[min(climk(1),clim1(1)) max(climk(2),clim1(2))];
    end
    if ~isinf(xScale)
    handle(k).XData = xFac*asinh(handle(k).XData/xScale);
    xlimk=[min(handle(k).XData(:)) max(handle(k).XData(:))];
    xlim1=[min(xlimk(1),xlim1(1)) max(xlimk(2),xlim1(2))];
    end
    if ~isinf(yScale)
    handle(k).YData = yFac*asinh(handle(k).YData/yScale);
    ylimk=[min(handle(k).YData(:)) max(handle(k).YData(:))];
    ylim1=[min(ylimk(1),ylim1(1)) max(ylimk(2),ylim1(2))];
    end
    if ~isinf(zScale)
    handle(k).ZData = zFac*asinh(handle(k).ZData/zScale);
    zlimk=[min(handle(k).ZData(:)) max(handle(k).ZData(:))];
    zlim1=[min(zlimk(1),zlim1(1)) max(zlimk(2),zlim1(2))];
    end
    handle(k).UserData = 'quasiLogAxes';
  end%for k
end%for kk
```

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.

```
if ~isinf(xScale),
    if xlim('mode')=="manual"
         xlim1=xFac*asinh(xlim0/xScale);
    else xlim1=xlim1+0.04*diff(xlim1)*[-1 1];
    end, end
if ~isinf(yScale),
    if ylim('mode')=="manual"
         ylim1=yFac*asinh(ylim0/yScale);
    else ylim1=ylim1+0.04*diff(ylim1)*[-1 1];
    end, end
if ~isinf(zScale),
    if zlim('mode')=="manual"
         zlim1=zFac*asinh(zlim0/zScale);
    else zlim1=zlim1+0.04*diff(zlim1)*[-1 1];
    end, end
if ~isinf(cScale),
    if theAxes.CLimMode=="manual"
         clim1=cFac*asinh(clim0/cScale);
    else clim1=clim1+   0*diff(clim1)*[-1 1];
    end, end
```

Scale axes, and tick marks on axes

```
if ~isinf(xScale)
    xlim(xlim1);
    tickingQuasiLogAxes(theAxes,'X',xlim1,xScale,xFac)
end%if
if ~isinf(yScale)
    ylim(ylim1);
    tickingQuasiLogAxes(theAxes,'Y',ylim1,yScale,yFac)
end%if
if ~isinf(zScale)
    zlim(zlim1);
    tickingQuasiLogAxes(theAxes,'Z',zlim1,zScale,zFac)
end%if
```

But for color, only tick when we find a colorbar.

```
if ~isinf(cScale)
  caxis(clim1);
  for p=1:numel(theFig.Children)
    ca = theFig.Children(p);
    if class(ca) == "matlab.graphics.illustration.ColorBar"
      tickingQuasiLogAxes(ca,'C',clim1,cScale,cFac)
      break
    end
  end
end%if
```

Turn the grid on by default.

```
grid on
end%function
```

3.20.1 `tickingQuasiLogAxes()`: typeset ticks and labels on an axis

```
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.

```
    qmax=max(abs(qlim1));
    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`).

```
    ticks=10.^(qmag+(-7:0));
    j=find(ticks>qScale*sinh(0.06*qmax/qFac));
    nj=length(j);
    if nj<3,     ticks=[1;2;5]*ticks(j);
    elseif nj<5, ticks=[1;3]*ticks(j);
    else         ticks=ticks(j);
    end
    ticks=sort([0;ticks(:);-ticks(:)]);
```

Set the ticks in place according to the transformation.

```
    if Q=='C', p='s'; Q=''; else p=''; end
    set(ca,[Q 'Tick' p],qFac*asinh(ticks/qScale) ...
          ,[Q 'TickLabel' p],cellstr(num2str(ticks,4)))
    if Q=='X', set(ca,[Q 'TickLabelRotation'],40), end
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.

```
clear all, close all
global patches
nRealise = 20
```

3.20.2.1 Check divided difference interpolation

```
fprintf('\n\n**** Check divided difference interpolation\n')
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.)

```
for iReal=1:nRealise
    nEdge = randi(3)% =1,2, or 3
    edgyInt = rand<0.5
    nSubP = nEdge*( (2-edgyInt)*randi(2)+1+edgyInt )
    ordCC = 2*randi(4)
    nPatch = ordCC+randi([2 4])
    Domain=5*[-rand rand]
    dx=rand*diff(Domain)/nPatch/nSubP
```

```
    configPatches1(@sin,Domain,'equispace',nPatch,ordCC,dx,nSubP ...
        ,'EdgyInt',edgyInt,'nEdge',nEdge);
    patches.intTest = true;
```

Displace patches to a random non-uniform spacing.

```
H = diff(patches.x(1,:,:,1:2));
patches.x = patches.x+0.8*H*(rand(1,1,1,nPatch)-0.5);
%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.

```
    ps=1:ordCC
    cs=randn(size(ps));
    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.

```
    u=u0;  u([1:nEdge  end-nEdge+1:end],:)=inf;
```

Then evaluate the interpolation and squeeze the singleton dimension of an 'ensemble'.

```
    ui=patchEdgeInt1(u(:));
    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.

```
    j=1:nPatch;
    iError=ui(:,:,j)-u0(:,:,j);
    hist(log10(abs(iError(abs(iError)>0))),-17:-9)
    xlabel('log10 iError'),pause(0.3)%??
    normError=norm(iError(:))
    assert(normError<1e-13*4^ordCC ...
    ,'failed divided difference interpolation')
```

End the for-loop over random parameters.

```
end%for iReal
fprintf('\n\nPassed all divided difference interpolation\n')
```

3.20.2.2 Test standard spectral interpolation

```
fprintf('\n\n**** Test standard spectral interpolation\n')
pause(1)
```

Test over random numbers of patches, random domain lengths, random microscale spacing, random choice of `edgyInt`. Say do fifteen realisations.

```
for iReal=1:nRealise
    nEdge=randi(3)% =1,2, or 3
    edgyInt = rand<0.5
    nSubP = nEdge*( (2-edgyInt)*randi(2)+1+edgyInt )
    nPatch=randi([5 10])
    Len=10*rand
    dx=0.5*rand*Len/nPatch/nSubP
    configPatches1(@sin,[0 Len],'periodic',nPatch,0,dx,nSubP ...
        ,'EdgyInt',edgyInt,'nEdge',nEdge); % random Edgy or not
    if mod(nPatch,2)==0, fprintf('\nAvoiding highest wavenumber\n'), end
    kMax=floor((nPatch-1)/2);
```

Test single field Set a profile, and evaluate the interpolation.

```
for k=-kMax:kMax
  u0=exp(1i*k*patches.x*2*pi/Len);
  u=u0;  u([1:nEdge  end-nEdge+1:end],:)=nan;
  ui=patchEdgeInt1(u(:));
  normError=rms(ui(:)-u0(:));
  if abs(normError)>5e-14
    normError=normError, k=k
    error(['failed single var interpolation k=' num2str(k)])
  end
end
```

Test multiple fields Use this to measure some of the errors in order to omit singleton dimensions,

```
  normDiff=@(u,v) ...
  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.

```
for k=1:(nPatch-1)/2 % not checking the highest wavenumber
  u0=sin(k*patches.x*2*pi/Len);
  v0=cos(k*patches.x*2*pi/Len);
  uvi=patchEdgeInt1( reshape([u0 v0],[],1) );
  normuError=normDiff(uvi(:,1,:,:),u0);
  normvError=normDiff(uvi(:,2,:,:),v0);
  if abs(normuError)+abs(normvError)>2e-13
    normuError=normuError, normvError=normvError
    error(['failed double field interpolation k=' num2str(k)])
  end
end
```

End the for-loop over various geometries.

```
end
fprintf('\nPassed standard spectral interpolation tests\n')
```

3.20.2.3 Now test spectral interpolation on staggered grid

```
fprintf('\n\n**** Test spectral interpolation on staggered\n')
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.

```
for iReal=1:nRealise
    nEdge = 1 % required
    edgyInt = rand<0.5
    nPatch=2*randi([3 10])
    nSubP=7 % of form 4*N-1
    Len=10*rand
    dx=0.5*rand*Len/nPatch/nSubP
    configPatches1(@simpleWavepde,[0 Len],'periodic' ...
        ,nPatch,-1,dx,nSubP,'EdgyInt',edgyInt,'nEdge',nEdge);
    if mod(nPatch,4)==0, fprintf('\nAvoiding highest wavenumber\n'), end
    kMax=floor((nPatch/2-1)/2)
```

Identify which microscale grid points are h or u values.

```
uPts=mod( (1:nSubP)'+(1:nPatch) ,2);
hPts=find(1-uPts);
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.

```
fprintf('Staggered: single field-pair test.\n')
for k=-kMax:kMax
  U0=nan(nSubP,nPatch);
  U0(hPts)=rand*exp(+1i*k*patches.x(hPts)*2*pi/Len);
  U0(uPts)=rand*exp(-1i*k*patches.x(uPts)*2*pi/Len);
  U=U0;
  U([1:nEdge  end-nEdge+1:end],:)=nan;
  Ui=patchEdgeInt1(U0(:));
  normError=norm(Ui(:)-U0(:));
  if abs(normError)>5e-14
    normError=normError
    patches=patches
    error(['staggered: failed single sys interpolation k=' num2str(k)])
  end
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).

```
  normDiff=@(u,v,w) ...
  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.

```
fprintf('Staggered: Two field-pairs test.\n')
x0=patches.x((nSubP+1)/2,1);
patches.x=patches.x-x0;
oddP=1:2:nPatch; evnP=2:2:nPatch;
for k=1:kMax
  U0=nan(nSubP,1,1,nPatch); V0=U0;
  U0(hPts)=rand*sin(k*patches.x(hPts)*2*pi/Len);
  U0(uPts)=rand*sin(k*patches.x(uPts)*2*pi/Len);
  U=U0; U([1:nEdge  end-nEdge+1:end],:)=nan;
  V0(hPts)=rand*cos(k*patches.x(hPts)*2*pi/Len);
  V0(uPts)=rand*cos(k*patches.x(uPts)*2*pi/Len);
  V=V0; V([1:nEdge  end-nEdge+1:end],:)=nan;
  UVi=patchEdgeInt1([U0 V0]);
  normuError=[normDiff(UVi(:,1,:,oddP),U0(:,:,:,oddP),U0(:,:,:,evnP))
      normDiff(UVi(:,1,:,evnP),U0(:,:,:,evnP),U0(:,:,:,oddP))]';
  normvError=[normDiff(UVi(:,2,:,oddP),V0(:,:,:,oddP),V0(:,:,:,evnP))
      normDiff(UVi(:,2,:,evnP),V0(:,:,:,evnP),V0(:,:,:,oddP))]';
  if norm(normuError)+norm(normvError)>2e-13
    normuError=normuError, normvError=normvError
    patches=patches
    error(['staggered: failed double field interpolation k=' num2str(k)])
  end
end
```

End for-loop over patches

```
end
```

3.20.2.4 Check standard finite width interpolation

```
fprintf('\n\n**** Check standard finite width interpolation\n')
pause(1)
```

Check over various types and orders of interpolation, numbers of patches, random domain lengths and random ratios. (The `@sin` is a dummy.)

```
for iReal=1:nRealise
    nEdge=randi(3)% =1,2, or 3
    edgyInt = rand<0.5
    nSubP = nEdge*( (2-edgyInt)*randi(2)+1+edgyInt )
    ordCC = 2*randi(4)
    nPatch = ordCC+randi([2 4])
    Domain=5*[-rand rand]
    dx=0.5*rand*diff(Domain)/nPatch/nSubP
    configPatches1(@sin,Domain,'periodic',nPatch,ordCC,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.

```
    ps=1:ordCC
    cs=randn(size(ps));
    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.

```
    u=u0;  u([1:nEdge  end-nEdge+1:end],:)=nan;
```

Then evaluate the interpolation and squeeze the singleton dimension of an 'ensemble'.

```
    ui=patchEdgeInt1(u(:));
    ui=squeeze(ui);
```

The interior patches should have zero error.

```
    j=ordCC/2+1:nPatch-ordCC/2;
    iError=ui(:,:,j)-u0(:,:,j);
    normError=norm(iError(:))
    assert(normError<5e-12 ...
    ,'failed finite stencil interpolation')
```

End the for-loops over various parameters.

```
end%for iReal
fprintf('\nPassed all standard polynomial interpolation\n')
```

3.20.2.5 Now test finite width interpolation on staggered grid

```
fprintf('\n\n**** Check finite width staggered\n')
pause(1)
```

Must have even number of patches for a staggered grid.

```
for iReal=1:nRealise
    nEdge = 1 % required for now
    edgyInt = rand<0.5
    nPatch=2*randi([3 10])
    nSubP=3; % of form 4*N-1
    Len=10*rand
    dx=0.5*rand*Len/nPatch/nSubP
    configPatches1(@simpleWavepde,[0 Len],'periodic' ...
        ,nPatch,-1,dx,nSubP,'EdgyInt',edgyInt,'nEdge',nEdge);
    kMax=floor((nPatch/2-1)/2)
```

Identify which microscale grid points are h or u values.

```
    uPts=mod( (1:nSubP)'+(1:nPatch) ,2);
    hPts=find(1-uPts);
    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.

```
fprintf('\nSingle field-pair test.\n')
for k=-kMax:kMax
  U0=nan(nSubP,nPatch);
  U0(hPts)=rand*exp(+1i*k*patches.x(hPts)*2*pi/Len);
  U0(uPts)=rand*exp(-1i*k*patches.x(uPts)*2*pi/Len);
  Ui=squeeze(patchEdgeInt1(U0(:)));
  normError=norm(Ui-U0);
  if abs(normError)>5e-14
    normError=normError
    error(['failed single sys interpolation k=' num2str(k)])
  end
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.

```
i0=(nSubP+1)/2; % centre-patch index
fprintf('Two field-pairs test.\n')
x0=patches.x((nSubP+1)/2,1);
patches.x=patches.x-x0;
for k=1:nPatch/4
  U0=nan(nSubP,1,1,nPatch); V0=U0;
  U0(hPts)=rand*sin(k*patches.x(hPts)*2*pi/Len);
  U0(uPts)=rand*sin(k*patches.x(uPts)*2*pi/Len);
  V0(hPts)=rand*cos(k*patches.x(hPts)*2*pi/Len);
  V0(uPts)=rand*cos(k*patches.x(uPts)*2*pi/Len);
  UVi=patchEdgeInt1([U0 V0]);
  Ui=squeeze(UVi(:,1,1,:));
  Vi=squeeze(UVi(:,2,1,:));
  normuError=norm(Ui(:,1:2:nPatch)-U0(:,1:2:nPatch))*norm(U0(i0,2:2:nPatch))
            +norm(Ui(:,2:2:nPatch)-U0(:,2:2:nPatch))*norm(U0(i0,1:2:nPatch));
  normvError=norm(Vi(:,1:2:nPatch)-V0(:,1:2:nPatch))*norm(V0(i0,2:2:nPatch))
            +norm(Vi(:,2:2:nPatch)-V0(:,2:2:nPatch))*norm(V0(i0,1:2:nPatch));
  if abs(normuError)+abs(normvError)>2e-13
    normuError=normuError, normvError=normvError
    error(['failed double field interpolation k=' num2str(k)])
  end
end
```

End for-loop over the realisations

```
end
```

3.20.2.6 Finish

If no error messages, then all OK.

```
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

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.

```
function patches = configPatches2(fun,Xlim,Dom ...
    ,nPatch,ordCC,dx,nSubP,varargin)
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)`] × [`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 $0, 2, 4, \ldots$; 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` $= \frac{1}{2}$ 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 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 `(nSubP-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]

```
if nargout==0, global patches, end
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 `.Cwtsl`, only for macro-periodic conditions, are the `ordCC` $\times$ 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)` $\times 1 \times 1 \times 1 \times$ `nPatch(1)` $\times 1$ 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

```
if nargin==0
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).

```
global patches
patches = configPatches2(@nonDiffPDE,[-3 3 -2 2] ...
    ,'periodic', [9 7], 0, 0.12, 5 ,'EdgyInt',false);
```

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

```
u0 = exp(-patches.x.^2-patches.y.^2);
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.

```
figure(1), clf, colormap(0.8*hsv)
x = squeeze(patches.x);  y = squeeze(patches.y);
if 1, x([1 end],:) = nan; y([1 end],:) = nan; end
```

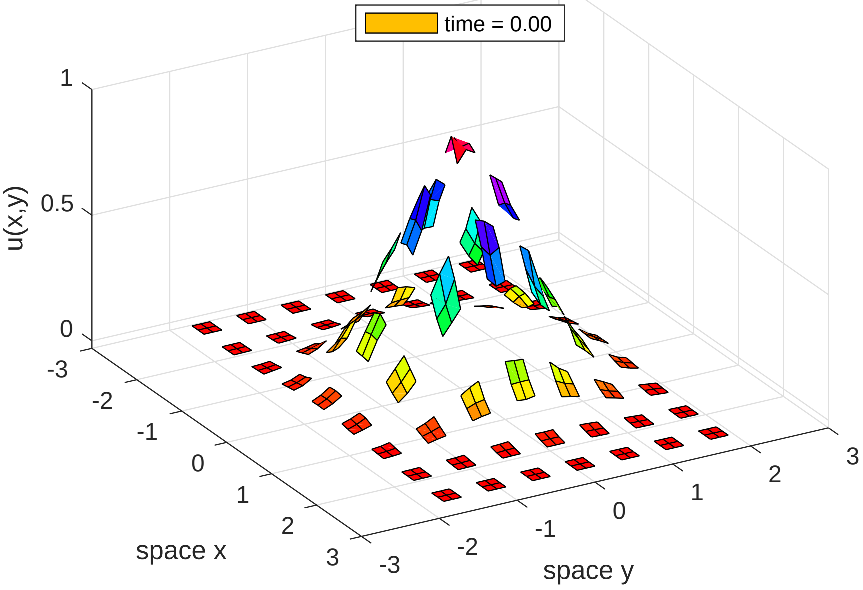
Start by showing the initial conditions of Figure 4.1 while the simulation computes.

```
u = reshape(permute(squeeze(u0) ...
    ,[1 3 2 4]), [numel(x) numel(y)]);
hsurf = mesh(x(:),y(:),u');
axis([-3 3 -3 3 -0.03 1]), view(60,40)
legend('time = 0.00','Location','north')
xlabel('space $x$'), ylabel('space $y$'), zlabel('$u(x,y)$')
colormap(hsv)
ifOurCf2eps([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.

```
disp('Wait to simulate nonlinear diffusion h_t=(h^3)_xx+(h^3)_yy')
drawnow
if ~exist('OCTAVE_VERSION','builtin')
    [ts,us] = ode23(@patchSys2,linspace(0,2).^2,u0(:));
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 $t = 3$.




```
    lsode_options('absolute tolerance',1e-4);
    lsode_options('relative tolerance',1e-4);
    [ts,us] = ode0cts(@patchSys2,[0 1],u0(:));
end
```

Animate the computed simulation to end with Figure 4.2. Use `patchEdgeInt2` to interpolate patch-edge values.

```
for i = 1:length(ts)
  u = patchEdgeInt2(us(i,:));
  u = reshape(permute(squeeze(u) ...
      ,[1 3 2 4]), [numel(x) numel(y)]);
  set(hsurf,'ZData', u');
  legend(['time = ' num2str(ts(i),'%4.2f')])
  pause(0.1)
end
ifOurCf2eps([mfilename 't3'])
```

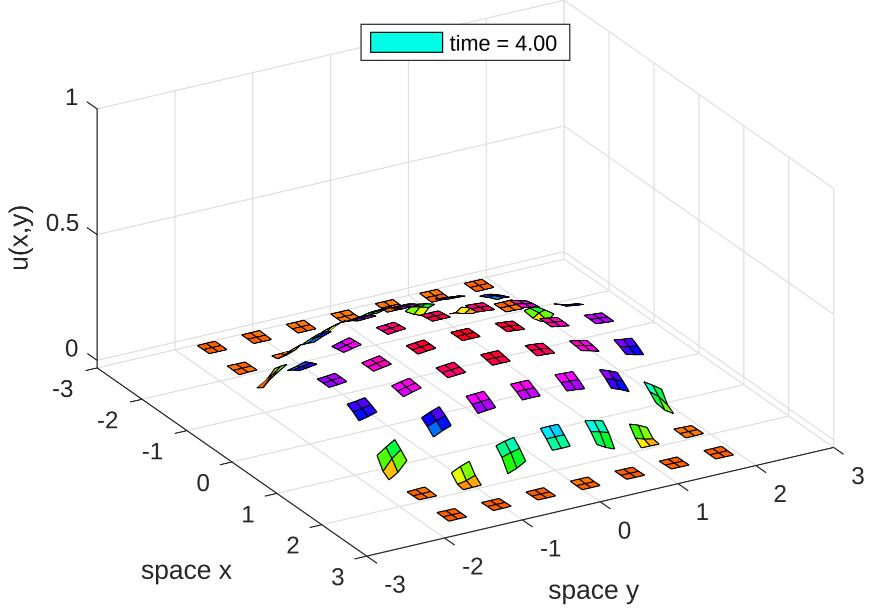
Upon finishing execution of the example, exit this function.

```
return
end%if no arguments
```

Example of nonlinear diffusion PDE inside patches As a microscale discretisation of $u_t = \nabla^2(u^3)$, code $\dot u_{ijkl} = \frac{1}{\delta x^2}(u^3_{i+1,j,k,l} - 2u^3_{i,j,k,l} + u^3_{i-1,j,k,l}) + \frac{1}{\delta y^2}(u^3_{i,j+1,k,l} - 2u^3_{i,j,k,l} + u^3_{i,j-1,k,l})$.

```
function ut = nonDiffPDE(t,u,patches)
  if nargin<3, global patches, end
  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.*




```
  dx = diff(patches.x(1:2));  % microgrid spacing
  dy = diff(patches.y(1:2));
  i = 2:size(u,1)-1;  j = 2:size(u,2)-1;  % interior patch points
  ut = nan+u;  % preallocate output array
  ut(i,j,:,:) = diff(u(:,j,:,:).^3,2,1)/dx^2 ...
               +diff(u(i,:,:,:).^3,2,2)/dy^2;
end
```

4.1.2 Parse input arguments and defaults

```
p = inputParser;
fnValidation = @(f) isa(f, 'function_handle');%test for fn name
addRequired(p,'fun',fnValidation);
addRequired(p,'Xlim',@isnumeric);
%addRequired(p,'Dom'); % nothing yet decided
addRequired(p,'nPatch',@isnumeric);
addRequired(p,'ordCC',@isnumeric);
addRequired(p,'dx',@isnumeric);
addRequired(p,'nSubP',@isnumeric);
addParameter(p,'nEdge',1,@isnumeric);
addParameter(p,'EdgyInt',false,@islogical);
addParameter(p,'nEnsem',1,@isnumeric);
addParameter(p,'hetCoeffs',[],@isnumeric);
addParameter(p,'parallel',false,@islogical);
%addParameter(p,'nCore',1,@isnumeric); % not yet implemented
parse(p,fun,Xlim,nPatch,ordCC,dx,nSubP,varargin{:});
```

Set the optional parameters.

```
patches.nEdge = p.Results.nEdge;
if numel(patches.nEdge)==1
    patches.nEdge = repmat(patches.nEdge,1,2);
    end
patches.EdgyInt = p.Results.EdgyInt;
patches.nEnsem = p.Results.nEnsem;
cs = p.Results.hetCoeffs;
patches.parallel = p.Results.parallel;
%patches.nCore = p.Results.nCore;
```

Initially duplicate parameters for both space dimensions as needed.

```
if numel(Xlim)==2,   Xlim = repmat(Xlim,1,2); end
if numel(nPatch)==1, nPatch = repmat(nPatch,1,2); end
if numel(dx)==1,     dx = repmat(dx,1,2); end
if numel(nSubP)==1,  nSubP = repmat(nSubP,1,2); end
```

Check parameters.

```
assert(Xlim(1)<Xlim(2) ...
      ,'first pair of Xlim must be ordered increasing')
assert(Xlim(3)<Xlim(4) ...
      ,'second pair of Xlim must be ordered increasing')
assert((mod(ordCC,2)==0)|all(patches.nEdge==1) ...
      ,'Cannot yet have nEdge>1 and staggered patch grids')
assert(all(3*patches.nEdge<=nSubP) ...
      ,'too many edge values requested')
assert(all(rem(nSubP,patches.nEdge)==0) ...
      ,'nSubP must be integer multiple of nEdge')
if ~patches.EdgyInt, assert(all(rem(nSubP./patches.nEdge,2)==1) ...
      ,'for non-edgyInt, nSubP./nEdge must be odd integer')
      end
if (patches.nEnsem>1)&all(patches.nEdge>1)
      warning('not yet tested when both nEnsem and nEdge non-one')
      end
%if patches.nCore>1
%    warning('nCore>1 not yet tested in this version')
%    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.

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

Default macroscale conditions are periodic with evenly spaced patches.

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

```
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.

```
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.

```
patches.periodic=false;
for p=1:2
switch Dom.type(p,:)
case 'periodic'
    patches.periodic=true;
    if isfield(Dom,'bcOffset')
    warning('bcOffset not available for Dom.type = periodic'), end
    msg=' not available for Dom.type = periodic';
    if isfield(Dom,'X'), warning(['X' msg]), end
    if isfield(Dom,'Y'), warning(['Y' msg]), end
case {'equispace','chebyshev'}
    if ~isfield(Dom,'bcOffset'), Dom.bcOffset=zeros(2,2); end
    % for mixed with usergiven, following should still work
    if numel(Dom.bcOffset)==1
        Dom.bcOffset=repmat(Dom.bcOffset,2,2); end
    if numel(Dom.bcOffset)==2
        Dom.bcOffset=repmat(Dom.bcOffset(:)',2,1); end
    msg=' not available for Dom.type = equispace or chebyshev';
    if (p==1)& isfield(Dom,'X'), warning(['X' msg]), end
    if (p==2)& isfield(Dom,'Y'), warning(['Y' msg]), end
case 'usergiven'
%    if isfield(Dom,'bcOffset')
%    warning('bcOffset not available for usergiven Dom.type'), end
    msg=' required for Dom.type = usergiven';
    if p==1, assert(isfield(Dom,'X'),['X' msg]), end
    if p==2, assert(isfield(Dom,'Y'),['Y' msg]), end
otherwise
    error([Dom.type ' is unknown Dom.type'])
end%switch Dom.type
end%for p
```

4.1.3 The code to make patches

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

```
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]

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

For odd `ordCC` do interpolation based upon odd neighbouring patches as is useful for staggered grids.

```
patches.stag = mod(ordCC,2);
assert(patches.stag==0,'staggered not yet implemented??')
ordCC = ordCC+patches.stag;
patches.ordCC = ordCC;
```

Check for staggered grid and periodic case.

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

```
for q=1:2
qq=2*q-1;
```

Distribution depends upon `Dom.type`:

```
switch Dom.type(q,:)
```

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

```
case 'periodic'
  Q=linspace(Xlim(qq),Xlim(qq+1),nPatch(q)+1);
  DQ=Q(2)-Q(1);
  Q=Q(1:nPatch(q))+diff(Q)/2;
  pEI=patches.EdgyInt; % abbreviation
  pnE=patches.nEdge(q);% abbreviation
  if pre2023, dx(q) = ratio(q)*DQ/(nSubP(q)-pnE*(1+pEI))*(2-pEI);
  else        ratio(q) = dx(q)/DQ*(nSubP(q)-pnE*(1+pEI))/(2-pEI);
  end
  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.

```
case 'equispace'
  Q=linspace(Xlim(qq)+((nSubP(q)-1)/2-Dom.bcOffset(qq))*dx(q) ...
          ,Xlim(qq+1)-((nSubP(q)-1)/2-Dom.bcOffset(qq+1))*dx(q) ...
```

[2] **ToDo:** Perhaps implement staggered spectral coupling.

```
          ,nPatch(q));
  DQ=diff(Q(1:2));
  width=(1+patches.EdgyInt)/2*(nSubP(q)-1-patches.EdgyInt)*dx;
  if DQ<width*0.999999
     warning('too many equispace patches (double overlapping)')
     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]

```
case 'chebyshev'
  halfWidth=dx(q)*(nSubP(q)-1)/2;
  Q1 = Xlim(1)+halfWidth-Dom.bcOffset(qq)*dx(q);
  Q2 = Xlim(2)-halfWidth+Dom.bcOffset(qq+1)*dx(q);
%  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`.

```
  pEI=patches.EdgyInt; % abbreviation
  pnE=patches.nEdge(q);% abbreviation
  width=(1+pEI)/2*(nSubP(q)-pnE*(1+pEI))*dx(q);
  for b=0:2:nPatch(q)-2
    DQmin=(Q2-Q1-b*width)/2*( 1-cos(pi/(nPatch(q)-b-1)) );
    if DQmin>width, break, end
  end%for
  if DQmin<width*0.999999
     warning('too many Chebyshev patches (mid-domain overlap)')
     end
```

Assign the centre-patch coordinates.

```
  Q =[ Q1+(0:b/2-1)*width ...
       (Q1+Q2)/2-(Q2-Q1-b*width)/2*cos(linspace(0,pi,nPatch(q)-b)) ...
       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.

```
case 'usergiven'
  if q==1, Q = reshape(Dom.X,1,[]);
  else     Q = reshape(Dom.Y,1,[]);
  end%if
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.

```
if q==1, X=Q; end
if q==2, Y=Q; end
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).

```
xs = dx(1)*( (1:nSubP(1))-mean(1:nSubP(1)) );
patches.x = reshape( xs'+X ...
                   ,nSubP(1),1,1,1,nPatch(1),1);
ys = dx(2)*( (1:nSubP(2))-mean(1:nSubP(2)) );
patches.y = reshape( ys'+Y ...
                   ,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]

```
if patches.periodic
  ratio = reshape(ratio,1,2); % force to be row vector
  patches.ratio=ratio;
  if ordCC>0
    [Cwtsr,Cwtsl] = patchCwts(ratio,ordCC,patches.stag);
    patches.Cwtsr = Cwtsr;  patches.Cwtsl = Cwtsl;
  end%if
end%if patches.periodic
```

4.1.4 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`. 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()`.

```
nE = patches.nEnsem;
patches.le = 1:nE;  patches.ri = 1:nE;
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 then 3D, then the higher-dimensions are reshaped into the 3rd dimension.

```
if ~isempty(cs)
  [mx,my,nc] = size(cs);
  nx = nSubP(1); ny = nSubP(2);
  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.

```
  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.

```
    patches.nEnsem = mx*my;
    patches.cs = nan(nx-1,ny-1,nc,mx,my);
    for j = 1:my
        js = (j:j+ny-2);
        for i = 1:mx
            is = (i:i+nx-2);
            patches.cs(:,:,:,i,j) = cs(is,js,:);
        end
    end
    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.

```
    le = mod((0:mx-1)+mod(nx-2,mx),mx)+1;
    patches.le = reshape(  le'+mx*(0:my-1)  ,[],1);
    ri = mod((0:mx-1)-mod(nx-2,mx),mx)+1;
    patches.ri = reshape(  ri'+mx*(0:my-1)  ,[],1);
    bo = mod((0:my-1)+mod(ny-2,my),my)+1;
    patches.bo = reshape( (1:mx)'+mx*(bo-1) ,[],1);
    to = mod((0:my-1)-mod(ny-2,my),my)+1;
    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]

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

[5] **ToDo:** Maybe need to justify this and the arbitrary threshold more carefully??

End the two if-statements.

```
  end%if-else nEnsem>1
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]

```
if patches.parallel
%  theparpool=gcp()
  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.

```
  [~,pari]=max(nPatch+0.01*(1:2));
  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.

```
  switch pari
    case 1, patches.x=codistributed(patches.x,patches.codist);
    case 2, patches.y=codistributed(patches.y,patches.codist);
  otherwise
    error('should never have bad index for parallel distribution')
  end%switch
  end%spmd
```

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

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

Fin

```
end% function
```

[6] If 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.

```
function dudt = patchSys2(t,u,patches,varargin)
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`×`nEsem`×`nPatch(1)`× `nPatch(2)`. Time derivatives must be computed into the same sized array, although herein the patch edge-values are overwritten by zeros.
  - `.x` is `nSubP(1)` × 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()`.

```
sizeu = size(u);
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.

```
dudt = patches.fun(t,u,patches,varargin{:});
m = patches.nEdge(1);
dudt([1:m end-m+1:end],:,:) = 0;
m = patches.nEdge(2);
dudt(:,[1:m end-m+1:end],:) = 0;
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`.

```
function u = patchEdgeInt2(u,patches)
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`$\times 1\times 1\times 1\times$`nPatch1`$\times 1$ 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 $1\times$ `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 $\{0, 2, 4, \ldots\}$
  - `.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, `nSubP1` · `nSubP2` · `nVars` · `nEnsem` · `nPatch1` · `nPatch2`, 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.

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

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

```
[~,ny,~,~,~,Ny] = size(patches.y);
[nx,~,~,~,Nx,~] = size(patches.x);
nEnsem = patches.nEnsem;
nVars = round(numel(u)/numel(patches.x)/numel(patches.y)/nEnsem);
assert(numel(u) == nx*ny*Nx*Ny*nVars*nEnsem ...
  ,'patchEdgeInt2: input u has wrong size for parameters')
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.

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

```
%x = patches.x;
%if patches.nEdge(1)>1
%  m = patches.nEdge(1);
%  x = x(1:m:nx,:,:,:,:,:);
%  nx = nx/m;
%  u = reshape(u,m,nx,ny,nVars,nEnsem,Nx,Ny);
%  nVars = nVars*m;
```

```
%  u = reshape( permute(u,[2:3 1 4:7]) ...
%              ,nx,ny,nVars,nEnsem,Nx,Ny);
%end%if patches.nEdge(1)
%y = patches.y;
%if patches.nEdge(2)>1
%  m = patches.nEdge(2);
%  y = y(:,1:m:ny,:,:,:,:);
%  ny = ny/m;
%  u = reshape(u,nx,m,ny,nVars,nEnsem,Nx,Ny);
%  nVars = nVars*m;
%  u = reshape( permute(u,[1 3 2 4:7]) ...
%              ,nx,ny,nVars,nEnsem,Nx,Ny);
%end%if patches.nEdge(2)
x = patches.x;
y = patches.y;
if mean(patches.nEdge)>1
  mx = patches.nEdge(1);
  my = patches.nEdge(2);
  x = x(1:mx:nx,:,:,:,:,:);
  y = y(:,1:my:ny,:,:,:,:);
  nx = nx/mx;
  ny = ny/my;
  u = reshape(u,mx,nx,my,ny,nVars,nEnsem,Nx,Ny);
  nVars = nVars*mx*my;
  u = reshape( permute(u,[2 4 1 3 5:8]) ...
             ,nx,ny,nVars,nEnsem,Nx,Ny);
end%if patches.nEdge
```

The centre of each patch (as `nx` and `ny` are odd for centre-patch interpolation) is at indices

```
i0 = round((nx+1)/2);
j0 = round((ny+1)/2);
```

4.3.1 Periodic macroscale interpolation schemes

```
if patches.periodic
```

Get the size ratios of the patches.

```
rx = patches.ratio(1);
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.

```
ordCC = patches.ordCC;
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.

```
  if patches.EdgyInt % interpolate next-to-face values
    U = u([2 nx-1],2:(ny-1),:,:,I,J);
  else % interpolate centre-cross values
    U = u(i0,2:(ny-1),:,:,I,J);
  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.

```
szUO=size(U); szUO=[szUO ones(1,6-length(szUO)) ordCC];
```

Use finite difference formulas for the interpolation, so store finite differences $(\mu\delta, \delta^2, \mu\delta^3, \delta^4, \ldots)$ in these arrays. When parallel, in order to preserve the distributed array structure we use an index at the end for the differences.

```
  if ~patches.parallel, dmu = zeros(szUO); % 7D
  else   dmu = zeros(szUO,patches.codist); % 7D
  end%if patches.parallel
```

First compute differences $\mu\delta$ and δ^2.

```
  if patches.stag % use only odd numbered neighbours
    error('polynomial interpolation not yet for staggered patch coupling')
%    dmux(:,:,:,:,I,:,1) = (Ux(:,:,:,:,Ip,:)+Ux(:,:,:,:,Im,:))/2; % \mu
%    dmux(:,:,:,:,I,:,2) = (Ux(:,:,:,:,Ip,:)-Ux(:,:,:,:,Im,:)); % \delta
%    Ip = Ip(Ip); Im = Im(Im); % increase shifts to \pm2
%    dmuy(:,:,:,:,:,J,1) = (Ux(:,:,:,:,:,Jp)+Ux(:,:,:,:,:,Jm))/2; % \mu
%    dmuy(:,:,:,:,:,J,2) = (Ux(:,:,:,:,:,Jp)-Ux(:,:,:,:,:,Jm)); % \delta
%    Jp = Jp(Jp); Jm = Jm(Jm); % increase shifts to \pm2
  else %disp('starting standard interpolation')
    dmu(:,:,:,:,I,:,1) = (U(:,:,:,:,Ip,:) ...
                         -U(:,:,:,:,Im,:))/2; %\mu\delta
    dmu(:,:,:,:,I,:,2) = (U(:,:,:,:,Ip,:) ...
       -2*U(:,:,:,:,I,:) +U(:,:,:,:,Im,:));   %\delta^2
  end% if patches.stag
```

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

```
  for k = 3:ordCC
    dmu(:,:,:,:,I,:,k) =     dmu(:,:,:,:,Ip,:,k-2) ...
    -2*dmu(:,:,:,:,I,:,k-2) +dmu(:,:,:,:,Im,:,k-2);
  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`.

```
k=1+patches.EdgyInt; % use centre or two edges
u(nx,2:(ny-1),:,patches.ri,I,:) ...
  = U(1,:,:,:,:,:)*(1-patches.stag) ...
  +sum( shiftdim(patches.Cwtsr(:,1),-6).*dmu(1,:,:,:,:,:,:) ,7);
u(1 ,2:(ny-1),:,patches.le,I,:,:) ...
  = U(k,:,:,:,:,:)*(1-patches.stag) ...
  +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.

```
  if patches.EdgyInt % interpolate next-to-face values
    U = u(:,[2 ny-1],:,:,I,J);
  else % interpolate centre-cross values
    U = u(:,j0,:,:,I,J);
  end;%if patches.EdgyInt
```

Adjoin extra dimension for the array of differences.

```
szU0=size(U); szU0=[szU0 ones(1,6-length(szU0)) ordCC];
```

Store finite differences ($\mu\delta, \delta^2, \mu\delta^3, \delta^4, \ldots$) in this array.

```
  if ~patches.parallel, dmu = zeros(szU0); % 7D
  else   dmu = zeros(szU0,patches.codist); % 7D
  end%if patches.parallel
```

First compute differences $\mu\delta$ and δ^2.

```
  if patches.stag % use only odd numbered neighbours
    error('polynomial interpolation not yet for staggered patch coupling')
  else  %disp('starting standard interpolation')
    dmu(:,:,:,:,:,J,1) = (U(:,:,:,:,:,Jp) ...
                         -U(:,:,:,:,:,Jm))/2; %\mu\delta
    dmu(:,:,:,:,:,J,2) = (U(:,:,:,:,:,Jp) ...
       -2*U(:,:,:,:,:,J) +U(:,:,:,:,:,Jm));   %\delta^2
  end% if stag
```

Recursively take δ^2.

```
  for k = 3:ordCC
    dmu(:,:,:,:,:,J,k) =     dmu(:,:,:,:,:,Jp,k-2) ...
    -2*dmu(:,:,:,:,:,J,k-2) +dmu(:,:,:,:,:,Jm,k-2);
  end
```

Interpolate macro-values using the weights pre-computed by `configPatches2()`. An ensemble of configurations may have cross-coupling.

```
k = 1+patches.EdgyInt; % use centre or two edges
u(:,ny,:,patches.to,:,J) ...
  = U(:,1,:,:,:,:)*(1-patches.stag) ...
  +sum( shiftdim(patches.Cwtsr(:,2),-6).*dmu(:,1,:,:,:,:,:) ,7);
u(:,1 ,:,patches.bo,:,J) ...
  = U(:,k,:,:,:,:)*(1-patches.stag) ...
  +sum( shiftdim(patches.Cwtsl(:,2),-6).*dmu(:,k,:,:,:,:,:) ,7);
```

4.3.1.2 Case of spectral interpolation

Assumes the domain is macro-periodic.

```
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 $\texttt{ks} = k2\pi/N$ for 'wavenumbers' $k = (0,1,\ldots,k_{\max},-k_{\max},\ldots,-1)$ for odd N, and $k = (0\,,1\,,\ldots,k_{\max}\,,\pm(k_{\max}+1)-k_{\max}\,,\ldots,-1)$ 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.

```
 if patches.stag % transform by doubling the number of fields
 error('staggered grid not yet implemented??')
   v=nan(size(u)); % currently to restore the shape of u
   u=cat(3,u(:,1:2:nPatch,:),u(:,2:2:nPatch,:));
   stagShift=reshape(0.5*[ones(nVars,1);-ones(nVars,1)],1,1,[]);
   iV=[nVars+1:2*nVars 1:nVars]; % scatter interp to alternate field
   r=r/2;           % ratio effectively halved
   nPatch=nPatch/2; % halve the number of patches
   nVars=nVars*2;   % double the number of fields
 else % the values for standard spectral
    stagShift = 0;
    iV = 1:nVars;
 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.

```
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, $k = (0\,, 1\,, \ldots\,, k_{\max}\,, +(k_{\max}+1) - k_{\max}\,, \ldots\,, -1)$.

```
  kMax = floor((Nx-1)/2);
  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`.

```
if ~patches.EdgyInt
     Cm = fft( u(i0,iy,:,:,:,:) ,[],5);
     Cp = Cm;
else
     Cm = fft( u(   2,iy ,:,patches.le,:,:) ,[],5);
     Cp = fft( u(nx-1,iy ,:,patches.ri,:,:) ,[],5);
end%if ~patches.EdgyInt
```

Now invert the Fourier transforms to complete interpolation. Enforce reality when appropriate.

```
u(nx,iy,:,:,:,:) = uclean( ifft( ...
    Cm.*exp(1i*(stagShift+kr))  ,[],5) );
u( 1,iy,:,:,:,:) = uclean( ifft( ...
    Cp.*exp(1i*(stagShift-kr))  ,[],5) );
```

y**-normal edge values** Set wavenumbers into a vector.

```
  kMax = floor((Ny-1)/2);
  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.

```
if ~patches.EdgyInt
     Cm = fft( u(:,j0,:,:,:,:) ,[],6);
     Cp = Cm;
else
     Cm = fft( u(:,2    ,:,patches.bo,:,:) ,[],6);
     Cp = fft( u(:,ny-1 ,:,patches.to,:,:) ,[],6);
end%if ~patches.EdgyInt
```

Invert the Fourier transforms to complete interpolation.

```
u(:,ny,:,:,:,:) = uclean( ifft( ...
    Cm.*exp(1i*(stagShift+kr))  ,[],6) );
u(:, 1,:,:,:,:) = uclean( ifft( ...
    Cp.*exp(1i*(stagShift-kr))  ,[],6) );
```

```
end% if ordCC>0 else, so spectral
```

4.3.2 Non-periodic macroscale interpolation

```
else% patches.periodic false
assert(~patches.stag, ...
'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.

```
if patches.ordCC<1
     px = Nx-1; py = Ny-1;
else px = min(patches.ordCC,Nx-1);
     py = min(patches.ordCC,Ny-1);
end
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]

```
  F = nan(patches.EdgyInt+1,ny-2,nVars,nEnsem,Nx,Ny,px+1);
  if patches.EdgyInt % interpolate next-to-edge values
    F(:,:,:,:,:,:,1) = u([nx-1 2],iy,:,:,:,:);
    X = x([nx-1 2],:,:,:,:,:);
  else % interpolate mid-patch cross-patch values
    F(:,:,:,:,:,:,1) = u(i0,iy,:,:,:,:);
    X = x(i0,:,:,:,:,:);
  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.

```
for q = 1:px
  i = 1:Nx-q;
  F(:,:,:,:,i,:,q+1) ...
  = (F(:,:,:,:,i+1 ,:,q)-F(:,:,:,:,i,:,q)) ...
  ./(X(:,:,:,:,i+q,:)   -X(:,:,:,:,i,:));
end
```

Interpolate with divided differences Now interpolate to find the edge-values on left/right edges at Xedge for every interior Y.

```
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.

```
  i = max(1,min(1:Nx,Nx-ceil(px/2))-floor(px/2));
  Uedge = F(:,:,:,:,i,:,px+1);
  for q = px:-1:1
    Uedge = F(:,:,:,:,i,:,q)+(Xedge-X(:,:,:,:,i+q-1,:)).*Uedge;
  end
```

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

```
u(1 ,iy,:,patches.le,:,:) = Uedge(1,:,:,:,:,:);
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.

```
  F = nan(nx,patches.EdgyInt+1,nVars,nEnsem,Nx,Ny,py+1);
  if patches.EdgyInt % interpolate next-to-edge values
    F(:,:,:,:,:,:,1) = u(:,[ny-1 2],:,:,:,:);
    Y = y(:,[ny-1 2],:,:,:,:);
  else % interpolate mid-patch cross-patch values
    F(:,:,:,:,:,:,1) = u(:,j0,:,:,:,:);
    Y = y(:,j0,:,:,:,:);
  end;
```

Form tables of divided differences.

```
for q = 1:py
  j = 1:Ny-q;
  F(:,:,:,:,:,j,q+1) ...
  = (F(:,:,:,:,:,j+1 ,q)-F(:,:,:,:,:,j,q)) ...
  ./(Y(:,:,:,:,:,j+q)   -Y(:,:,:,:,:,j));
end
```

Interpolate to find the edge-values on top/bottom edges `Yedge` for every x.

```
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.

```
  j = max(1,min(1:Ny,Ny-ceil(py/2))-floor(py/2));
  Uedge = F(:,:,:,:,:,j,py+1);
  for q = py:-1:1
    Uedge = F(:,:,:,:,:,j,q)+(Yedge-Y(:,:,:,:,:,j+q-1)).*Uedge;
  end
```

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

```
u(:,1 ,:,patches.bo,:,:) = Uedge(:,1,:,:,:,:);
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`.

```
if isfield(patches,'intTest')&&patches.intTest
else % usual case
    u( 1,:,:,:, 1,:) = nan;
    u(nx,:,:,:,Nx,:) = nan;
    u(:, 1,:,:,:, 1) = nan;
    u(:,ny,:,:,:,Ny) = nan;
end%if
```

End of the non-periodic interpolation code.

```
end%if patches.periodic else
```

Unfold multiple edges No need to restore x, y.

```
if mean(patches.nEdge)>1
  nVars = nVars/(mx*my);
  u = reshape( u ,nx,ny,mx,my,nVars,nEnsem,Nx,Ny);
  nx = nx*mx;
  ny = ny*my;
  u = reshape( permute(u,[3 1 4 2 5:8]) ...
             ,nx,ny,nVars,nEnsem,Nx,Ny);
end%if patches.nEdge
```

Fin, returning the 6D array of field values with interpolated edges.

```
end% function patchEdgeInt2
```

4.4 `wave2D`: example of a wave on patches in 2D

Section contents

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 $\leftrightarrow$ patchSys2 $\leftrightarrow$ 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.

```
global patches
nSubP = 5;
nPatch = 9;
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.

```
disp('Check linear stability of the wave scheme')
uv0 = zeros(nSubP,nSubP,2,1,nPatch,nPatch);
uv0([1 end],:,:,:,:,:) = nan;
uv0(:,[1 end],:,:,:,:) = nan;
i = find(~isnan(uv0));
```

Now construct the Jacobian. Since this is a *linear* wave PDE, use large perturbations.

```
small = 1;
jac = nan(length(i));
sizeJacobian = size(jac)
for j = 1:length(i)
  uv = uv0(:);
  uv(i(j)) = uv(i(j))+small;
```

```
  tmp = patchSys2(0,uv)/small;
  jac(:,j) = tmp(i);
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.

```
evals = eig(jac);
nEvals = length(evals)
[~,k] = sort(-abs(real(evals)));
evalsWithBiggestRealPart = evals(k(1:10))
if abs(real(evals(k(1))))>1e-4
    warning('eigenvalue failure: real-part > 1e-4')
    return, end
```

Check that the eigenvalues are close to true waves of the PDE (not yet the micro-discretised equations).

```
kwave = 0:(nPatch-1)/2;
freq = sort(reshape(sqrt(kwave'.^2+kwave.^2),1,[]));
freq = freq(diff([-1 freq])>1e-9);
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 u0 and v0 are in the form required for computation: $n_x \times n_y \times 1 \times 1 \times N_x \times N_y$.

```
u0 = exp(-patches.x.^2-patches.y.^2);
v0 = zeros(size(u0));
```

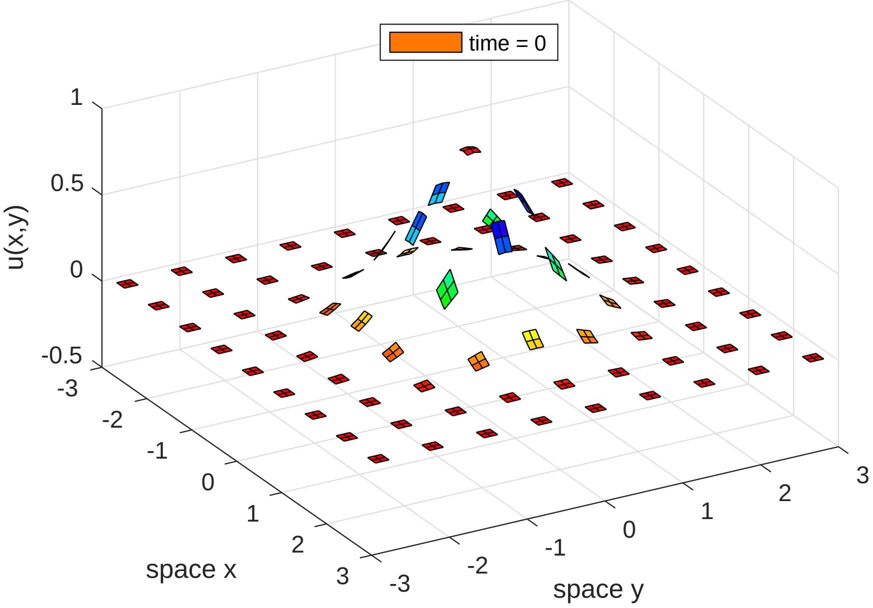
Initiate a plot of the simulation using only the microscale values interior to the patches: set x and y-edges to nan to leave the gaps. Start by showing the initial conditions of Figure 4.1 while the simulation computes. To mesh/surf plot we need to ?? 'transpose' to size $n_x \times N_x \times n_y \times N_y$, then reshape to size $n_x \cdot N_x \times n_y \cdot N_y$.

```
x = squeeze(patches.x); y = squeeze(patches.y);
x([1 end],:) = nan; y([1 end],:) = nan;
u = reshape(permute(squeeze(u0),[1 3 2 4]), [numel(x) numel(y)]);
usurf = surf(x(:),y(:),u');
axis([-3 3 -3 3 -0.5 1]), view(60,40)
xlabel('space $x$'), ylabel('space $y$'), zlabel('$u(x,y)$')
legend('time = 0','Location','north')
colormap(hsv)
drawnow
ifOurCf2eps([mfilename 'ic'])
```

Integrate in time using standard functions.

```
disp('Wait while we simulate u_t=v, v_t=u_xx+u_yy')
uv0 = cat(3,u0,v0);
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 $t = 2$.*




```
[ts,uvs] = ode23( @patchSys2,[0 6],uv0(:));
else % octave version is slower
[ts,uvs] = odeOcts(@patchSys2,linspace(0,6),uv0(:));
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.

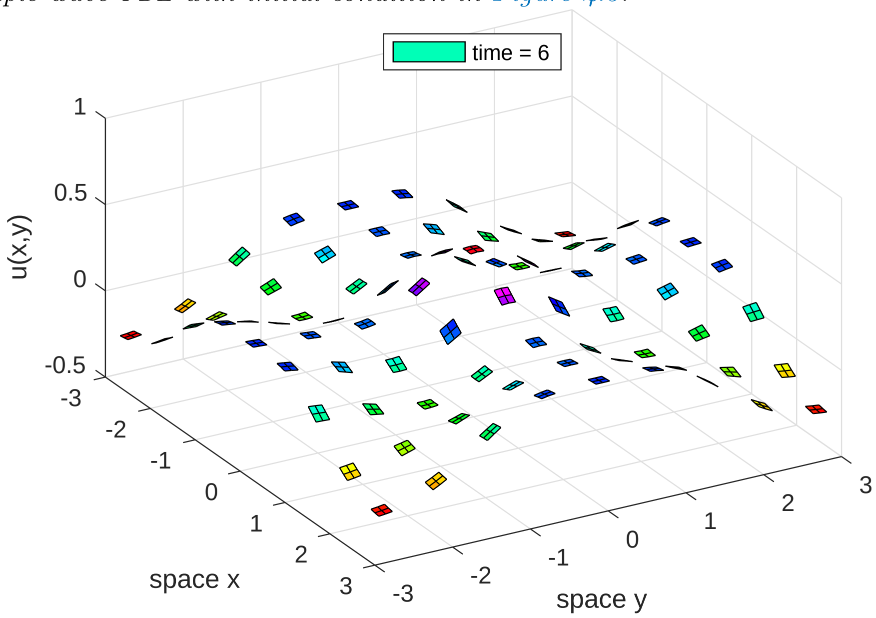
```
di = ceil(length(ts)/100);
for i = [1:di:length(ts)-1 length(ts)]
  uv = patchEdgeInt2(uvs(i,:));
  uv = reshape(permute(uv,[1 5 2 6 3 4]), [numel(x) numel(y) 2]);
  set(usurf,'ZData', uv(:,:,1)');
  legend(['time = ' num2str(ts(i),2)])
  pause(0.1)
end
ifOurCf2eps([mfilename 't' num2str(ts(end))])
```

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 $\dot v_{ijkl} = \frac{1}{\delta x^2}(u_{i+1,j,k,l} - 2u_{i,j,k,l} + u_{i-1,j,k,l}) + \frac{1}{\delta y^2}(u_{i,j+1,k,l} - 2u_{i,j,k,l} + u_{i,j-1,k,l})$.

```
function uvt = wavePDE(t,uv,patches)
  dx = diff(patches.x(1:2));
  dy = diff(patches.y(1:2));  % microscale spacing
  i = 2:size(uv,1)-1;
  j = 2:size(uv,2)-1; % interior patch-points
  uvt = nan+uv;  % preallocate storage
  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.*




```
  uvt(i,j,2,:) = diff(uv(:,j,1,:),2,1)/dx^2 ...
                +diff(uv(i,:,1,:),2,2)/dy^2;
end
```

```
function [ts,xs] = odeOcts(dxdt,tSpan,x0)
    if length(tSpan)>2, ts = tSpan;
    else ts = linspace(tSpan(1),tSpan(end),21)';
    end
    lsode_options('integration method','non-stiff');
    xs = lsode(@(x,t) dxdt(t,x),x0,ts);
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.

```
mPeriod = randi([2 3],1,2)
cHetr = exp(1*randn([mPeriod 2]));
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.

```
edgyInt = true;
nEnsem = 1 %prod(mPeriod) % or just set one
if nEnsem==1% use more patches
    nPatch = [9 9]
    nSubP = (2-edgyInt)*mPeriod+1+edgyInt
else % when nEnsem>1 use fewer patches
    nPatch = [5 5]
    nSubP = mPeriod+randi([1 4],1,2) % +2 is decoupled
end
ratio = 0.2+0.2*rand(1,2)
configPatches2(@heteroDiff2,[-pi pi -pi pi],nan,nPatch ...
    ,0,ratio,nSubP ,'EdgyInt',edgyInt ,'nEnsem',nEnsem ...
    ,'hetCoeffs',cHetr );
```

Simulate Set initial conditions of a simulation, replicated for each in the ensemble.

```
global patches
u0 = 0.8*cos(patches.x).*sin(patches.y) ...
     +0.1*randn([nSubP,1,1,nPatch]);
u0 = repmat(u0,1,1,1,nEnsem,1,1);
```

Integrate using standard integrators, unevenly spaced in time to better display transients.

```
if ~exist('OCTAVE_VERSION','builtin')
    [ts,us] = ode23(@patchSys2, 0.3*linspace(0,1).^2, u0(:));
else % octave version
    [ts,us] = odeOcts(@patchSys2, 0.3*linspace(0,1).^2, u0(:));
end
```

Plot the solution as an animation over time.

```
if ts(end)>0.099, disp('plot animation of solution field')
figure(1), clf, colormap(hsv)
```

Get spatial coordinates and pad them with NaNs to separate patches.

```
x = squeeze(patches.x); y = squeeze(patches.y);
x(end+1,:)=nan;  y(end+1,:)=nan; % pad with nans
```

For every time step draw the surface and pause for a short display.

```
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.

```
  u = squeeze( mean( patchEdgeInt2(us(i,:)) ,4));
  u(end+1,:,:,:)=nan; u(:,end+1,:,:)=nan;
  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.

```
  if i==1
       hsurf = surf(x(:),y(:),u'); view(60,40)
       axis([-pi pi -pi pi -1 1]),   caxis([-1 1])
       xlabel('$x$'), ylabel('$y$'), zlabel('$u(x,y)$')
  else set(hsurf,'ZData', u');
  end
  legend(['time = ' num2str(ts(i),2)],'Location','north')
  pause(0.05)
```

finish the animation loop and if-plot.

```
end%for over time
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.

```
ratio = [0.1 0.1]
nLeadEvals=prod(nPatch)+max(nPatch);
leadingEvals=[];
```

Evaluate eigenvalues for spectral as the base case for polynomial interpolation of order $2, 4, \ldots$.

```
maxords=10;
for ord=0:2:maxords
    ord=ord
```

Configure with same parameters, then because they are reset by this configuration, restore coupling.

```
    configPatches2(@heteroDiff2,[-pi pi -pi pi],nan,nPatch ...
        ,ord,ratio,nSubP,'EdgyInt',edgyInt,'nEnsem',nEnsem ...
        ,'hetCoeffs',cHetr);
```

Find which elements of the 6D array are interior micro-grid points and hence correspond to dynamical variables.

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

Construct the Jacobian of the scheme as the matrix of the linear transformation, obtained by transforming the standard unit vectors.

```
    jac = nan(length(i));
    sizeJacobian = size(jac)
    for j = 1:length(i)
      u = u0(:)+(i(j)==(1:numel(u0))');
      tmp = patchSys2(0,u);
      jac(:,j) = tmp(i);
    end
```

Test for symmetry, with error if we know it should be symmetric.

```
    notSymmetric=norm(jac-jac')
    if edgyInt, assert(notSymmetric<1e-7,'failed symmetry')
    elseif notSymmetric>1e-7, disp('failed symmetry')
    end
```

Find all the eigenvalues (as `eigs` is unreliable).

```
    if edgyInt, [evecs,evals] = eig((jac+jac')/2,'vector');
    else evals = eig(jac);
    end
    biggestImag=max(abs(imag(evals)));
    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.

```
    [~,k] = sort(-real(evals));
    evals=evals(k); evecs=evecs(:,k);
    if ord==0, nZeroEv=sum(abs(evals(:))<1e-5), end
    if ord==0, evec0=evecs(:,1:nZeroEv*nLeadEvals);
    else % find evec closest to that of each leading spectral
        [~,k]=max(abs(evecs'*evec0));
        evals=evals(k); % sort in corresponding order
    end
    leadingEvals=[leadingEvals evals(nZeroEv*(1:nLeadEvals))];
end
```

```
disp('     spectral    quadratic      quartic  sixth-order ...')
leadingEvals=leadingEvals
```

Plot the errors in the eigenvalues using the spectral ones as accurate. Only plot every second, `iEv`, as all are repeated eigenvalues.

```
if maxords>2
    iEv=2:2:12;
    figure(2);
    err=abs(leadingEvals-leadingEvals(:,1)) ...
        ./(1e-7+abs(leadingEvals(:,1)));
    semilogy(2:2:maxords,err(iEv,2:end)','o:')
    xlabel('coupling order')
    ylabel('eigenvalue relative error')
    leg=legend( ...
        strcat('$',num2str(real(leadingEvals(iEv,1)),'%.4f'),'$') ...
        ,'Location','northeastoutside');
    if ~exist('OCTAVE_VERSION','builtin')
        title(leg,'eigenvalues'), end
    legend boxoff
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^x_{ij} and c^y_{ij}, have previously been stored in `patches.cs` (3D).

```
function ut = heteroDiff2(t,u,patches)
  dx = diff(patches.x(2:3));  % x space step
  dy = diff(patches.y(2:3));  % y space step
  ix = 2:size(u,1)-1; % x interior points in a patch
  iy = 2:size(u,2)-1; % y interior points in a patch
  ut = nan+u;         % preallocate output array
  ut(ix,iy,:,:,:,:) ...
  = diff(patches.cs(:,iy,1,:).*diff(u(:,iy,:,:,:,:),1),1)/dx^2 ...
   +diff(patches.cs(ix,:,2,:).*diff(u(ix,:,:,:,:,:),1,2),1,2)/dy^2;
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.

```
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.

```
mPeriod = round(128*epsilon) %round(1024*epsilon)
```

So the migro-grid spacing is exactly

```
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 $\pi y/\epsilon$.

```
cHetr=[];
v=pi*(  1:mPeriod)/mPeriod;
h=pi*(0.5:mPeriod)/mPeriod;
cHetr(:,:,1) = 1+100*cos(h').^2*sin(v).^2;
cHetr(:,:,2) = 1+100*cos(v').^2*sin(h).^2;
```

Plot surfaces of the diffusivity.

```
figure(2),surf(h/pi,v/pi,cHetr(:,:,2))
hold on,  surf(v/pi,h/pi,cHetr(:,:,1))
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.

```
nPatch = [8 8]
H = 2./nPatch
HepsilonRatio = H/epsilon
```

Best when each patch spans an integral number of periods plus one grid step. The smallest such patches are

```
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.

```
ratio = ((nSubP-2)*dx)./H
```

Specify spectral interpolation. The edgy interpolation is self-adjoint (Bunder et al. 2020) leading to a symmetric matrix problem.

```
configPatches2(@hetDiffForce2,[-1 1 -1 1],nan,nPatch ...
    ,0,ratio,nSubP ,'EdgyInt',true  ...
    ,'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.

```
global patches i
u0 = zeros([nSubP,1,1,nPatch]);
u0([1 end],:,:) = nan; u0(:,[1 end],:) = nan;
i = find(~isnan(u0));
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.

```
tic;
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.

```
else
    maxIt = ceil(nVars/10);
    rhsb = theRes(u0(i));
    uSoln = pcg(@(u) rhsb-theRes(u),rhsb,1e-9,maxIt);
end
solnTime = toc
```

Store the solution into the patches, and give magnitudes.

```
u0(i) = uSoln;
normSoln = norm(uSoln)
normResidual = norm(theRes(uSoln))
```

Draw solution profile First reshape arrays to suit 2D space surface plots.

```
figure(1), clf, colormap(hsv)
x = squeeze(patches.x); y = squeeze(patches.y);
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.

```
surf(x(:),y(:),u'); view(60,40)
maxu = ceil(max(u(:))*10)/10;
axis([0 1 0 1 0 maxu]),   caxis([0 maxu])
xlabel('$x$'), ylabel('$y$'), zlabel('$u(x,y)$')
```

Assess errors in the patch scheme Invoke the function with desired interpolation: 0, spectral; $2, 4, \ldots$, polynomial.

```
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 derivativeat each point in the interior of a patch, output in `ut`. The two 2D array of diffusivities, c^x_{ij} and c^y_{ij}, are stored in `patches.cs` (3D).

```
function ut = hetDiffForce2(t,u,patches)
  dx = diff(patches.x(2:3));  % x space step
  dy = diff(patches.y(2:3));  % y space step
  ix = 2:size(u,1)-1; % x interior points in a patch
  iy = 2:size(u,2)-1; % y interior points in a patch
  ut = nan+u;         % preallocate output array
  fu = -u+100*sin(pi*patches.x).*sin(pi*patches.y);
  ut(ix,iy,:,:,:,:) ...
  = diff(patches.cs(:,iy,1).*diff(u(:,iy,:,:,:,:),1),1)/dx^2 ...
   +diff(patches.cs(ix,:,2).*diff(u(ix,:,:,:,:,:),1,2),1,2)/dy^2 ...
   +fu(ix,iy,:,:,:,:);
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.

```
function f=theRes(u)
  global i patches
  v=nan(size(patches.x+patches.y));
  v(i)=u;
  f=patchSys2(0,v(:),patches);
  f=f(i);
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 $2, 4, \ldots$ for corresponding polynomial interpolation schemes.

```
function errorsPatchScheme(ord)
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.

```
kMax = 3
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.

```
mPeriod = 9
```

So the migro-grid spacing is

```
dx = epsilon/mPeriod
```

Diffusivities Now form one period of the heterogeneity diffusivities exactly as in above code.

```
cHetr=[];
v=pi*(  1:mPeriod)/mPeriod;
h=pi*(0.5:mPeriod)/mPeriod;
cHetr(:,:,1) = 1+100*cos(h').^2*sin(v).^2;
cHetr(:,:,2) = 1+100*cos(v').^2*sin(h).^2;
```

Loop over different patch spacings

```
for k=1:kMax
nPatch = [2 2]*3^k
```

Patch configuration Zero-Dirichlet BCs on $(0, 1)^2$ are more-or-less encompassed by implementing periodic BCs on $(-1, 1)^2$.

```
H = 2./nPatch
HepsilonRatio = H/epsilon
```

Best when each patch spans an integral number of periods plus one grid step. The smallest such patches are

```
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.

```
ratio = ((nSubP-2)*dx)./H
```

The edgy interpolation leads to a symmetric matrix problem (Bunder et al. 2020).

```
configPatches2(@hetDiffForce2,[-1 1 -1 1],nan,nPatch ...
    ,ord,ratio,nSubP ,'EdgyInt',true  ...
    ,'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.

```
global patches i
u0 = zeros([nSubP,1,1,nPatch]);
u0([1 end],:,:) = nan; u0(:,[1 end],:) = nan;
i = find(~isnan(u0));
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.

```
tic
rhsb = theRes(u0(i));
uSoln = pcg(@(u) rhsb-theRes(u),rhsb,1e-6,999);
solnTime = toc
```

Store the solution into the patches, and trace magnitudes.

```
u0(i) = uSoln;
normSoln = norm(uSoln)
normResidual = norm(theRes(uSoln))
```

End loop over different patch spacings Store 4D field values in cell array for post-processing.

```
us{k}=squeeze(u0);
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.

```
disp('**** Relate errors for different patch spacing ****')
if ord==0, disp('**** Spectral interpolation between patches')
else disp(['**** Polynomial interpolation, order ' num2str(ord)])
```

```
end
i=2:nSubP-1;
I{1}=1:3;
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.

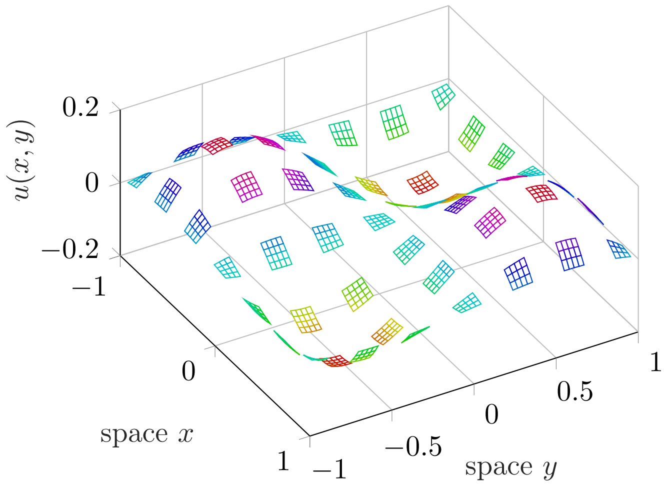
```
rmsError=[]; errorRatios=[]; orderInH=[];
for k=1:kMax-1
  error{k}=us{k}(i,i,I{k},I{k})-us{kMax}(i,i,I{kMax},I{kMax});
  rmsError(:,:,k)=squeeze(rms(rms(error{k})));
  if (k>1)&(ord>0)
    errorRatios(:,:,k-1)=rmsError(:,:,k)./rmsError(:,:,k-1);
    orderInH(:,:,k-1)=-log(errorRatios(:,:,k-1))/log(3);
  end
end
```

Display the results, and end the function.

```
rmsError=rmsError
errorRatios=errorRatios
orderInH=orderInH
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

$$A := \begin{bmatrix} 2 & a \\ a & 2 \end{bmatrix} \quad \text{with } a := \operatorname{sign}(xy) \text{ or } a := \sin(\pi x)\sin(\pi y),$$

and for forcing $f(x, y)$ such that the exact equilibrium is $u = x\big(1-e^{1-|x|}\big)y\big(1-e^{1-|y|}\big)$. 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.

```
clear all
global patches
%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

```
nPatch = 7
nSubP = 5
dx = 0.03
```

Specify some order of interpolation.

```
configPatches2(@monoscaleDiffForce2,[-1 1 -1 1],'equispace' ...
    ,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.

```
x=patches.x;  y=patches.y;
patches.A = sin(pi*x).*sin(pi*y);
patches.fu = ...
    +2*patches.A.*(9*x.^2.*y.^2-3*x.^2-3*y.^2+1) ...
    +12*x.*y.*(x.^2+y.^2-2);
```

By construction, the PDE has analytic solution

```
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.

```
u0 = zeros(nSubP,nSubP,1,1,nPatch,nPatch);
u0([1 end],:,:) = nan;  u0(:,[1 end],:) = nan;
patches.i = find(~isnan(u0));
nVariables = numel(patches.i)
```

Solve by iteration. Use `fsolve` for simplicity and robustness (using `optimoptions` to omit its trace information), and give magnitudes.

```
tic;
uSoln = fsolve(@theRes,u0(patches.i) ...
        ,optimoptions('fsolve','Display','off'));
solnTime = toc
normResidual = norm(theRes(uSoln))
normSoln = norm(uSoln)
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.

```
u0(patches.i) = uSoln;
u0 = patchEdgeInt2(u0);
```

Draw solution profile Separate patches with NaNs, then reshape arrays to suit 2D space surface plots.

```
figure(1), clf, colormap(0.8*hsv)
x(end+1,:,:)=nan;  u0(end+1,:,:)=nan;
```

```
y(:,end+1,:)=nan;  u0(:,end+1,:)=nan;
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.

```
mesh(x(:),y(:),u'); view(60,55)
xlabel('space $x$'), ylabel('space $y$'), zlabel('$u(x,y)$')
ifOurCf2tex(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`.

```
function ut = monoscaleDiffForce2(t,u,patches)
  dx = diff(patches.x(2:3));  % x space step
  dy = diff(patches.y(2:3));  % y space step
  i = 2:size(u,1)-1; % x interior points in a patch
  j = 2:size(u,2)-1; % y interior points in a patch
  ut = nan+u;         % preallocate output array
```

Set Dirichlet boundary value of zero around the square domain.

```
  u( 1 ,:,:,:, 1 ,:)=0; % left edge of left patches
  u(end,:,:,:,end,:)=0; % right edge of right patches
  u(:, 1 ,:,:,:, 1 )=0; % bottom edge of bottom patches
  u(:,end,:,:,:,end)=0; % top edge of top patches
```

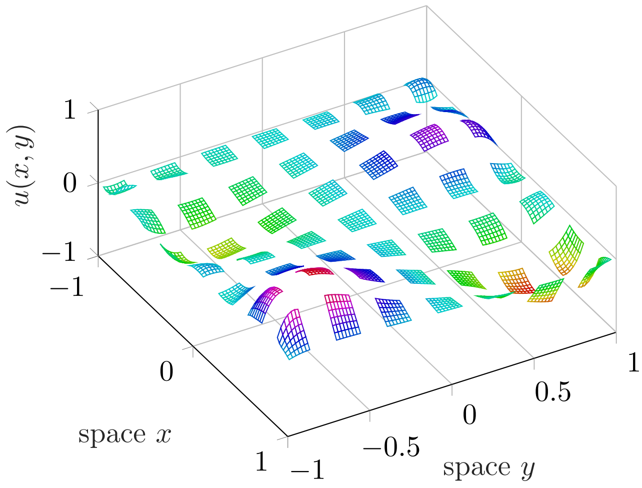
Or code some function variation around the boundary, such as a function of y on the left boundary, and a (constant) function of x at the top boundary.

```
  if 0
    u(1,:,:,:,1,:)=(1+patches.y)/2; % left edge of left patches
    u(:,end,:,:,:,end)=1; % top edge of top patches
  end%if
```

Compute the time derivatives via stored forcing and coefficients. Easier to code by conflating the last four dimensions into the one `,:`.

```
  ut(i,j,:) ...
  = 2*diff(u(:,j,:),2,1)/dx^2 +2*diff(u(i,:,:),2,2)/dy^2 ...
   +2*patches.A(i,j,:).*( u(i+1,j+1,:) -u(i-1,j+1,:) ...
     -u(i+1,j-1,:) +u(i-1,j-1,:) )/(4*dx*dy) ...
   -patches.fu(i,j,:);
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.

```
clear all
global patches
%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.

```
mPeriod = 6
z = (0.5:mPeriod)'/mPeriod;
A = sin(2*pi*z).*sin(2*pi*z');
```

Set the periodicity, via ϵ, and other microscale parameters.

```
nPeriodsPatch = 1 % any integer
epsilon = 2^(-6) % 4 or 5 to see the patches
dx = (2*epsilon)/mPeriod
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':

```
nPatch = 7
configPatches2(@twoscaleDiffForce2,[-1 1],'equispace' ...
    ,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.

```
x = patches.x;  y = patches.y;
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.

```
u0 = zeros(nSubP,nSubP,1,1,nPatch,nPatch);
u0([1 end],:,:) = nan;  u0(:,[1 end],:) = nan;
patches.i = find(~isnan(u0));
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.

```
tic;
uSoln = fsolve(@theRes,u0(patches.i) ...
        ,optimoptions('fsolve','Display','off'));
solveTime = toc
normResidual = norm(theRes(uSoln))
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.

```
u0(patches.i) = uSoln;
u0 = patchEdgeInt2(u0);
```

Draw solution profile Separate patches with NaNs, then reshape arrays to suit 2D space surface plots.

```
figure(1), clf, colormap(0.8*hsv)
x(end+1,:,:)=nan;  u0(end+1,:,:)=nan;
y(:,end+1,:)=nan;  u0(:,end+1,:)=nan;
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.

```
mesh(x(:),y(:),u'); view(60,55)
xlabel('space $x$'), ylabel('space $y$'), zlabel('$u(x,y)$')
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`.

```
function ut = twoscaleDiffForce2(t,u,patches)
  dx = diff(patches.x(2:3));  % x space step
  dy = diff(patches.y(2:3));  % y space step
  i = 2:size(u,1)-1; % x interior points in a patch
  j = 2:size(u,2)-1; % y interior points in a patch
  ut = nan+u;         % preallocate output array
```

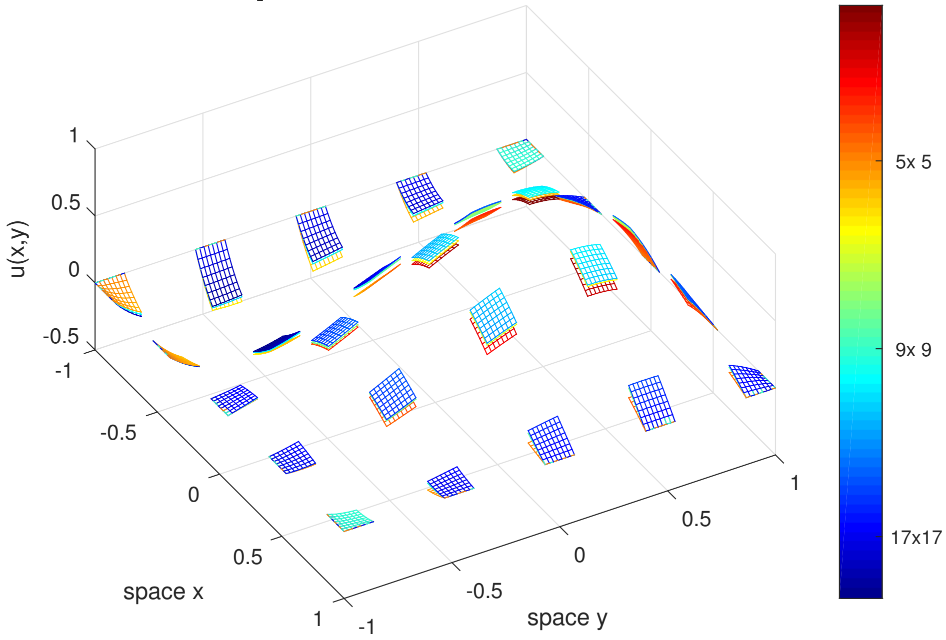
Set Dirichlet boundary value of zero around the square domain.

```
  u( 1 ,:,:,:, 1 ,:)=0; % left edge of left patches
  u(end,:,:,:,end,:)=0; % right edge of right patches
  u(:, 1 ,:,:,:, 1 )=0; % bottom edge of bottom patches
  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 `,:`.

```
  ut(i,j,:) ...
  = 2*diff(u(:,j,:),2,1)/dx^2 +2*diff(u(i,:,:),2,2)/dy^2 ...
   +2*patches.cs(i,j).*( u(i+1,j+1,:) -u(i-1,j+1,:) ...
     -u(i+1,j-1,:) +u(i-1,j-1,:) )/(4*dx*dy) ...
   -patches.fu(i,j,:);
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 twoscale 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

$$A := \begin{bmatrix} 2 & a \\ a & 2 \end{bmatrix} \quad \text{with } a := \sin(\pi x/\epsilon)\sin(\pi y/\epsilon),$$

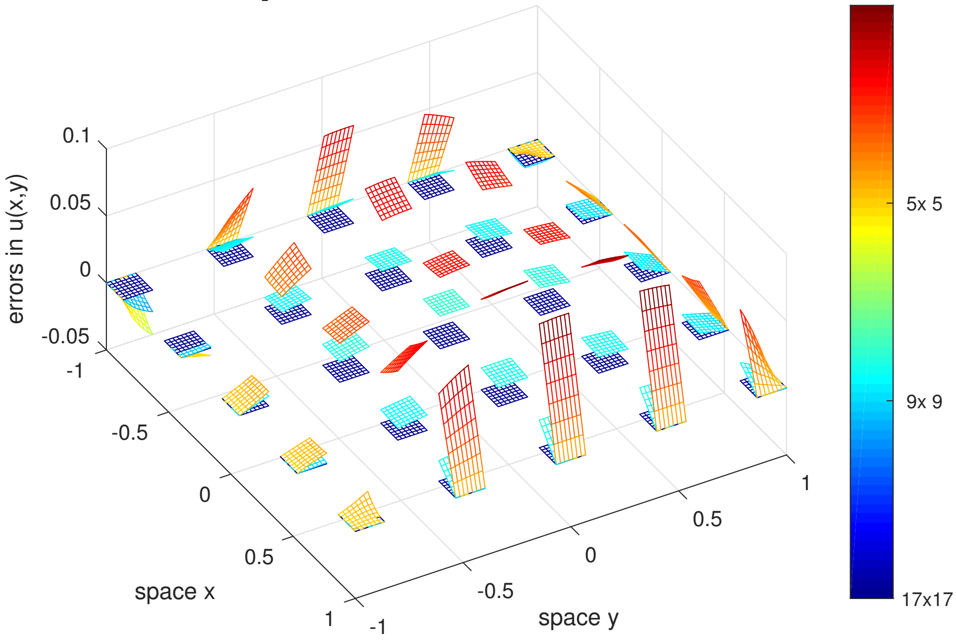
and for forcing $f := 10(x + y + \cos \pi x)$ (for which the solution has magnitude up to one).[12]

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).

```
clear all
global patches
%global OurCf2eps, OurCf2eps=true %option to save plot
switch 1
    case 1, Dom.type = 'equispace'
    case 2, Dom.type = 'chebyshev'
    case 3, Dom.type = 'usergiven'
end% switch
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.

```
mPeriod = 6
z = (0.5:mPeriod)'/mPeriod;
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:

```
log2Nmax = 4 % >2 up to 6 OKish
nPatchMax=2^log2Nmax+1
```

Set the periodicity ϵ, and other microscale parameters.

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

```
us=[]; xs=[]; ys=[]; nPs=[];
for log2N=log2Nmax:-1:2
    if log2N==log2Nmax
         Ps=linspace(1,nPatchMax ...
           ,5-2*all(Dom.type=='chebyshev'))
    else Ps=(Ps+1)/2
    end
```

Set the number of patches in $(-1, 1)$:

```
    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).

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

Configure the patches:

```
    configPatches2(@twoscaleDiffForce2,[-1 1],Dom,nPatch  ...
        ,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.

```
if 1
  patches.fu = 10*(patches.x+cos(pi*patches.x)+patches.y);
else patches.fu = 8+0*patches.x+0*patches.y;
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.

```
if log2N==log2Nmax
     u0 = zeros(nSubP,nSubP,1,1,nPatch,nPatch);
else u0 = u0(:,:,:,:,1:2:end,1:2:end);
end
u0([1 end],:,:) = nan;  u0(:,[1 end],:) = nan;
patches.i = find(~isnan(u0));
nVariables = numel(patches.i)
```

First try to solve via iterative solver `bicgstab`, via the generic patch system wrapper `theRes` (Section 3.19).

```
tic;
maxIt = ceil(nVariables/10);
rhsb = theRes( zeros(size(patches.i)) );
[uSoln,flag] = bicgstab(@(u) rhsb-theRes(u),rhsb ...
               ,1e-9,maxIt,[],[],u0(patches.i));
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.

```
if flag>0, disp('**** bicg failed, trying ILU preconditioner')
    disp(['Computing Jacobian: wait roughly ' ...
          num2str(nPatch^4/4500,2) ' secs'])
    tic
    Jac=sparse(nVariables,nVariables);
    for j=1:nVariables
        Jac(:,j)=sparse( rhsb-theRes((1:nVariables)'==j) );
    end
    formJacTime=toc
```

Compute an incomplete LU-factorization, and use it as preconditioner to `bicgstab`.

```
    tic
    [L,U] = ilu(Jac,struct('type','ilutp','droptol',1e-4));
    LUfillFactor = (nnz(L)+nnz(U))/nnz(Jac)
```

```
        [uSoln,flag] = bicgstab(@(u) rhsb-theRes(u),rhsb ...
                     ,1e-9,maxIt,L,U,u0(patches.i));
        precondSolveTime=toc
        assert(flag==0,'preconditioner fails bicgstab. Lower droptol?')
    end%if flag
```

Store the solution into the patches, and give magnitudes—Inf norm is max(abs()).

```
    normResidual = norm(theRes(uSoln),Inf)
    normSoln = norm(uSoln,Inf)
    u0(patches.i) = uSoln;
    u0 = patchEdgeInt2(u0);
    u0( 1 ,:,:,:, 1 ,:)=0; % left edge of left patches
    u0(end,:,:,:,end,:)=0; % right edge of right patches
    u0(:, 1 ,:,:,:, 1 )=0; % bottom edge of bottom patches
    u0(:,end,:,:,:,end)=0; % top edge of top patches
    assert(normResidual<1e-5,'poor--bad solution found')
```

Concatenate the solution on common patches into stores.

```
    us=cat(5,us,squeeze(u0(:,:,:,:,Ps,Ps)));
    xs=cat(3,xs,squeeze(patches.x(:,:,:,:,Ps,:)));
    ys=cat(3,ys,squeeze(patches.y(:,:,:,:,:,Ps)));
    nPs = [nPs;nPatch];
```

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').

```
end%for log2N
assert(max(abs(reshape(diff(xs,1,3),[],1)))<1e-12,'x-coord failure')
assert(max(abs(reshape(diff(ys,1,3),[],1)))<1e-12,'y-coord failure')
errs = us-us(:,:,:,:,1);
meanAbsErrs = mean(abs(reshape(errs,[],size(us,5))))
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.

```
x = xs(:,:,1); y = ys(:,:,1); u=us;
x(end+1,:)=nan;   y(end+1,:)=nan;
u(end+1,:,:)=nan; u(:,end+1,:)=nan;
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.

```
figure(1), clf, colormap(jet)
for p=1:size(u,3)
     mesh(x(:),y(:),u(:,:,p)',p+u(:,:,p)');
     hold on;
```

```
end, hold off
view(60,55)
colorbar('Ticks',1:size(u,3) ...
    ,'TickLabels',[num2str(nPs) ['x';'x';'x'] num2str(nPs)]);
xlabel('space $x$'), ylabel('space $y$'), zlabel('$u(x,y)$')
ifOurCf2eps([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.

```
err=u(:,:,1)-u;
maxAbsErr=max(abs(err(:)));
figure(2), clf, colormap(jet)
for p=1:size(u,3)
     mesh(x(:),y(:),err(:,:,p)',p+err(:,:,p)'/maxAbsErr);
     hold on;
end, hold off
view(60,55)
colorbar('Ticks',1:size(u,3) ...
    ,'TickLabels',[num2str(nPs) ['x';'x';'x'] num2str(nPs)]);
xlabel('space $x$'), ylabel('space $y$')
zlabel('errors in $u(x,y)$')
ifOurCf2eps(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`.

```
function ut = twoscaleDiffForce2(t,u,patches)
  dx = diff(patches.x(2:3));  % x space step
  dy = diff(patches.y(2:3));  % y space step
  i = 2:size(u,1)-1; % x interior points in a patch
  j = 2:size(u,2)-1; % y interior points in a patch
  ut = nan+u;         % preallocate output array
```

Set Dirichlet boundary value of zero around the square domain.

```
  u( 1 ,:,:,:, 1 ,:)=0; % left edge of left patches
  u(end,:,:,:,end,:)=0; % right edge of right patches
  u(:, 1 ,:,:,:, 1 )=0; % bottom edge of bottom patches
  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 `,:`.

```
  ut(i,j,:) ...
  = 2*diff(u(:,j,:),2,1)/dx^2 +2*diff(u(i,:,:),2,2)/dy^2 ...
   +2*patches.cs(i,j).*( u(i+1,j+1,:) -u(i-1,j+1,:) ...
```

```
      -u(i+1,j-1,:) +u(i-1,j-1,:) )/(4*dx*dy) ...
    +patches.fu(i,j,:);
end%function twoscaleDiffForce2
```

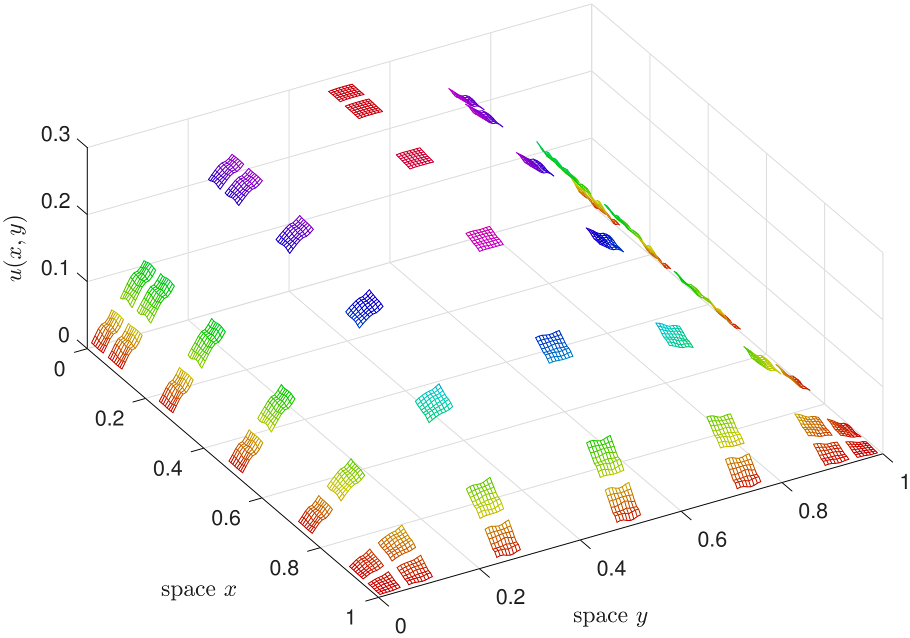


Figure 4.9: Equilibrium of the macroscale diffusion problem of Abdulle with boundary conditions of Dirichlet zero-value except for $x = 0$ which is Neumann (Section 4.10). Here the patches have a Chebyshev-like spatial distribution. The patch size is chosen large enough to see within.

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.

```
clear all
global patches
%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.)

```
mPeriod = 6
x = (0.5:mPeriod)'/mPeriod;  y=x';
a = (2+1.8*sin(2*pi*x))./(2+1.8*sin(2*pi*y)) ...
   +(2+    sin(2*pi*y))./(2+1.8*sin(2*pi*x));
diffusivityRange = [min(a(:)) max(a(:))]
```

Set the periodicity ϵ, here big enough so we can see the patches, and other microscale parameters.

```
epsilon = 0.04
dx = epsilon/mPeriod
nPeriodsPatch = 1 % any integer
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

```
Dom.bcOffset = zeros(2);
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':

```
nPatch = 7
Dom.type='chebyshev';
configPatches2(@abdulleDiffForce2,[0 1],Dom ...
    ,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.

```
u0 = zeros(nSubP,nSubP,1,1,nPatch,nPatch);
u0([1 end],:,:) = nan;  u0(:,[1 end],:) = nan;
patches.i = find(~isnan(u0));
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.

```
tic;
uSoln = fsolve(@theRes,u0(patches.i) ...
       ,optimoptions('fsolve','Display','off'));
solnTime = toc
normResidual = norm(theRes(uSoln))
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.

```
u0(patches.i) = uSoln;
u0 = patchEdgeInt2(u0);
```

Draw solution profile Separate patches with NaNs, then reshape arrays to suit 2D space surface plots.

```
figure(1), clf, colormap(0.8*hsv)
patches.x(end+1,:,:)=nan;  u0(end+1,:,:)=nan;
patches.y(:,end+1,:)=nan;  u0(:,end+1,:)=nan;
u = reshape(permute(squeeze(u0),[1 3 2 4]) ...
    , [numel(patches.x) numel(patches.y)]);
```

Draw the patch solution surface, with boundary-values omitted as already `NaN` by not bothering to set them.

```
mesh(patches.x(:),patches.y(:),u'); view(60,55)
xlabel('space $x$'), ylabel('space $y$'), zlabel('$u(x,y)$')
ifOurCf2eps(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`.

```
function ut = abdulleDiffForce2(t,u,patches)
  dx = diff(patches.x(2:3));  % x space step
  dy = diff(patches.y(2:3));  % y space step
  i = 2:size(u,1)-1; % x interior points in a patch
  j = 2:size(u,2)-1; % y interior points in a patch
  ut = nan+u;        % preallocate output array
```

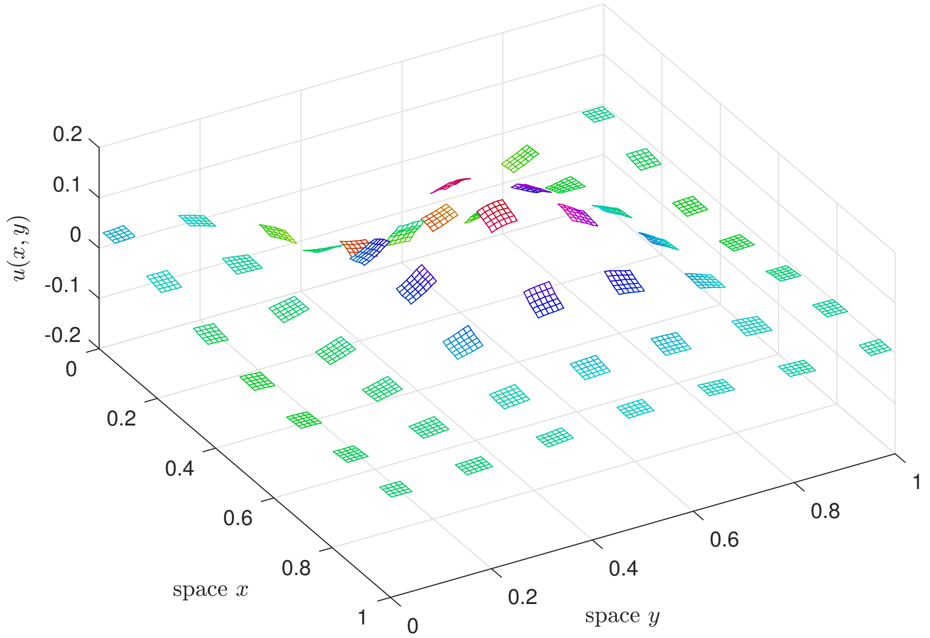
Set Dirichlet boundary value of zero around the square domain, but also cater for zero Neumann condition on the left boundary.

```
  u( 1 ,:,:,:, 1 ,:)=0; % left edge of left patches
  u(end,:,:,:,end,:)=0; % right edge of right patches
  u(:, 1 ,:,:,:, 1 )=0; % bottom edge of bottom patches
  u(:,end,:,:,:,end)=0; % top edge of top patches
  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 `,:`.

```
  ut(i,j,:) = diff(patches.cs(:,j).*diff(u(:,j,:)))/dx^2 ...
      + diff(patches.cs(i,:).*diff(u(i,:,:),1,2),1,2)/dy^2 ...
      + 10;
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.

```
clear all
global patches
%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.

```
mPeriod = 4
mu1 = 0.01*10.^rand(mPeriod)
mu2 = 2*pi*rand(mPeriod)
cs = cat(3,mu1,cos(mu2),sin(mu2));
meanDiffAdvec=squeeze(mean(mean(cs)))
```

Set the periodicity ϵ, here big enough so we can see the patches, and other microscale parameters.

```
epsilon = 0.04
dx = epsilon/mPeriod
nPeriodsPatch = 1 % any integer
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:

```
nPatch = 7
Dom.type= 'equispace';
Dom.bcOffset = 0.5;
configPatches2(@randAdvecDiffForce2,[0 1],Dom ...
    ,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.

```
mu = [ 0.25+0.5*rand(1,2) 0.1+0.15*rand ]
patches.fu = exp(-((patches.x-mu(1)).^2 ...
                  +(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.

```
u0 = zeros(nSubP,nSubP,1,1,nPatch,nPatch);
u0([1 end],:,:) = nan;  u0(:,[1 end],:) = nan;
patches.i = find(~isnan(u0));
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).

```
tic;
uSoln = fsolve(@theRes,u0(patches.i) ...
        ,optimoptions('fsolve','Display','off'));
solnTime = toc
```

```
normResidual = norm(theRes(uSoln))
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.

```
u0(patches.i) = uSoln;
u0 = patchEdgeInt2(u0);
```

Draw solution profile Separate patches with NaNs, then reshape arrays to suit 2D space surface plots.

```
figure(1), clf, colormap(0.8*hsv)
patches.x(end+1,:,:)=nan;  u0(end+1,:,:)=nan;
patches.y(:,end+1,:)=nan;  u0(:,end+1,:)=nan;
u = reshape(permute(squeeze(u0),[1 3 2 4]) ...
    , [numel(patches.x) numel(patches.y)]);
```

Draw the patch solution surface, with boundary-values omitted as already `NaN` by not bothering to set them.

```
mesh(patches.x(:),patches.y(:),u'); view(60,55)
xlabel('space $x$'), ylabel('space $y$'), zlabel('$u(x,y)$')
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`.

```
function ut = randAdvecDiffForce2(t,u,patches)
  dx = diff(patches.x(2:3));  % x space step
  dy = diff(patches.y(2:3));  % y space step
  i = 2:size(u,1)-1; % x interior points in a patch
  j = 2:size(u,2)-1; % y interior points in a patch
  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.

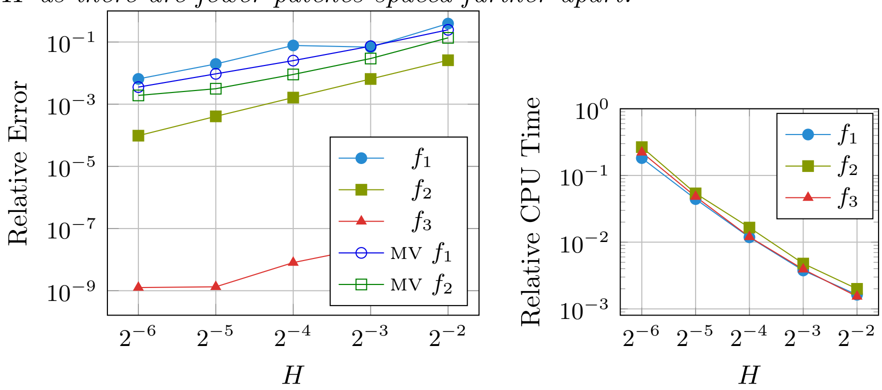
```
  u( 1 ,:,:,:, 1 ,:)=u(  2  ,:,:,:, 1 ,:); % left edge of left patches
  u(end,:,:,:,end,:)=u(end-1,:,:,:,end,:); % right edge of right patches
  u(:, 1 ,:,:,:, 1 )=u(:,  2  ,:,:,:, 1 ); % bottom edge of bottom patches
  u(:,end,:,:,:,end)=u(:,end-1,:,:,:,end); % top edge of top patches
```

Compute the time derivatives via stored forcing and coefficients. Easier to code by conflating the last four dimensions into the one `,:`.

```
  ut(i,j,:) ...
  = patches.cs(i,j,1).*(diff(u(:,j,:),2,1)/dx^2 ...
                       +diff(u(i,:,:),2,2)/dy^2)...
   -patches.cs(i,j,2).*(u(i+1,j,:)-u(i-1,j,:))/(2*dx) ...
```

```
    -patches.cs(i,j,3).*(u(i,j+1,:)-u(i,j-1,:))/(2*dy) ...
    -u(i,j,:) +patches.fu(i,j,:);
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 that 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.

```
clear all
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.

```
epsilon = 4*dx
nPeriodsPatch = 1
mPeriod = round(epsilon/dx)
nSubP = mPeriod*nPeriodsPatch+2
```

Choose which of three forcing functions to use

```
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.

```
nPatch = 2/epsilon/nPeriodsPatch
for iPat=0:9
if iPat>0, nPatch=nPatch/2, end
if nPatch<8, break, end
```

Set the periodic heterogeneous coefficient, isotropic:

$$a_\epsilon(t,x) = \big[3+\sin(2\pi x/\epsilon)+\sin(2\pi t)\big]\cdot\big[3+\sin(2\pi y/\epsilon)+\sin(2\pi t)\big],$$

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.

```
ratio = (nSubP-2)*dx/(2/nPatch)
Xleft=(1-ratio)/nPatch;
xmid=Xleft+dx*(0:mPeriod-1)';    % half-points
xi = Xleft+dx*(-0.5:mPeriod-1)'; % grid-points
% two components for ax, the x-dirn interactions
cHetr(:,:,1) = (3+cos(2*pi*xmid/epsilon))+0*xi';
cHetr(:,:,2) = 0*xmid+(3+cos(2*pi*xi'/epsilon));
% two components for ay, the y-dirn interactions
cHetr(:,:,3) = (3+cos(2*pi*xi/epsilon))+0*xmid';
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.

```
configPatches2(@heteroWave2,[-1 1 -1 1],nan,nPatch ...
    ,0,ratio,nSubP ,'EdgyInt',true ,'hetCoeffs',cHetr );
```

A check on the spatial geometry.

```
global patches
dxPat=diff(patches.x(1:2));
assert(abs(dx-dxPat)<1e-9,"dx mismatch")
```

Simulate Set the particular forcing function to use, and the zero initial conditions of a simulation.

```
patches.eff=fn;
clear uv0
uv0(:,:,1,1,:,:) = 0*patches.x+0*patches.y;
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`.

```
disp('Now simulate over time')
tic
[ts,us] = ode23(@patchSys2, linspace(0,1,11), uv0(:));
if iPat==0,  odeTime0=toc
else relOdeTime(iPat)=toc/odeTime0
end
```

Compute error compared to full domain simulation Get spatial coordinates of patch-interior points, and reshape to column vectors.

```
i = 2:nSubP-1;
x = squeeze(patches.x(i,:,:,:,:,:));
y = squeeze(patches.y(:,i,:,:,:,:));
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.

```
uv = squeeze( patchEdgeInt2(us(end,:)));
u = squeeze( uv(i,i,1,:,:) );
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.

```
if iPat==0
  x0=x; y0=y; u0=u;
```

```
  rms0=sqrt(mean(u0(:).^2))
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.

```
  [i,k] = find(abs(x0-x')<1e-9);
  assert(length(i)==length(x),'find error in index i')
  [j,k] = find(abs(y0-y')<1e-9);
  assert(length(j)==length(y),'find error in index j')
```

The RMS error over the surface is

```
  errs=u-u0(i,j);
  relrmserr(iPat)=sqrt(mean(errs(:).^2))/rms0
  H(iPat)=2/nPatch
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.

```
end%for iPat
figure(1), clf
loglog(H,relrmserr,'o:'),  grid on
xlabel('$H$'), ylabel('relative error')
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.

```
function ut = heteroWave2(t,u,patches)
  if nargin<3, global patches, end
```

Microscale space-steps, and interior point indices.

```
  dx = diff(patches.x(2:3));  % x micro-scale step
  dy = diff(patches.y(2:3));  % y micro-scale step
  i = 2:size(u,1)-1; % x interior points in a patch
  j = 2:size(u,2)-1; % y interior points in a patch
  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 $y = \pm 1$.

```
x=patches.x; y=patches.y;
l=find(abs(x)>1); x(l)=x(l)-sign(x(l))*2;
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.

```
f1 = ( (abs(x)>0.4)*(20*t+230*t^2) ...
      +(abs(x)<0.4)*(100*t+2300*t^2) ).*sign(x).*sign(y);
f2 = 20*t*x.*(1-abs(x)).*y.*(1-abs(y)) ...
    +230*t^2*(sign(y).*x.*(1-abs(x))+sign(x).*y.*(1-abs(y)));
f3 = (5*t+50*t^2)*sin(pi*x).*sin(pi*y);
```

Also set the heterogeneous interactions at this time.

```
ax = (patches.cs(:,:,1)+sin(2*pi*t)) ...
   .*(patches.cs(:,:,2)+sin(2*pi*t));
ay = (patches.cs(:,:,3)+sin(2*pi*t)) ...
   .*(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.

```
  ut = nan+u;  % preallocate output array
  ut(i,j,1,:) = u(i,j,2,:);
  ut(i,j,2,:) ...
  = diff(ax(:,j).*diff(u(:,j,1,:),1),1)/dx^2 ...
   +diff(ay(i,:).*diff(u(i,:,1,:),1,2),1,2)/dy^2 ...
   +(patches.eff==1)*f1(i,j,:,:) ...
   +(patches.eff==2)*f2(i,j,:,:) ...
   +(patches.eff==3)*f3(i,j,:,:) ...
   + 1e-4*(diff(u(:,j,2,:),2,1)/dx^2+diff(u(i,:,2,:),2,2)/dy^2);
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

Section contents

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

$$\partial_t u = -(1 + \nabla^2/k_0^2)^2 u + \mathrm{Ra}\, u - u^3, \tag{4.1}$$

with various boundary conditions at $x, y = 0, L$. For Ra just above critical, say $\mathrm{Ra} = 0.1$, 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 $\sqrt{\mathrm{Ra}}$, 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).

```
clear all
cMap=jet(64); cMap=0.8*cMap(7:end-7,:); % set colormap
basename = ['r' num2str(floor(1e5*rem(now,1))) mfilename]
%global OurCf2eps, OurCf2eps=true %optional to save plots
Ra = 0.2 % Ra>0 leads to patterns
nGapFac = 2
waveLength = 0.5/nGapFac
nPtsPeriod = 6
dx = waveLength/nPtsPeriod
k0 = 2.1*pi/waveLength
```

The above factor 2.1 is close to $3/\sqrt{2} = 2.1213$ for which $(\pm1, \pm2)$ modes have same linear growth-rate as $(\pm2, 0)$ 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.

```
nPatch = 5
nSubP = 2*nPtsPeriod+4
Len = nPatch;
ordCC = 4;
dom.type='equispace';
dom.bcOffset=[0.5 0.5;1.0 1.5]
patches = configPatches2(@SwiftHohenbergPDE,[0 Len],dom ...
    ,nPatch,ordCC,dx,nSubP,'EdgyInt',true,'nEdge',2);
xs=squeeze(patches.x);
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.

```
fprintf('\n**** Simulate in time\n')
u0 = 0.3*( -1+2*rand(size(patches.x+patches.y)) );
Ts=400*linspace(0,1,97).^2;
tic
[ts,us] = ode23(@patchSys2, Ts, u0(:),[],patches,k0,Ra);
simulateTime = toc
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.

```
xs([1:2 end-1:end],:) = nan;
ys([1:2 end-1:end],:) = nan;
us = reshape( permute(us,[1 3 2 4 5]) ...
            ,nSubP*nPatch,nSubP*nPatch,[]);
uRange=[min(us(:)) max(us(:))];
```

Second, plot six examples of the evolving pattern, equi-spaced in time-index.

```
plots = round( 1+linspace(0,1,7)*(numel(ts)-1) )
for p=2:numel(plots)
  figure(p),clf
  mesh(xs(:),ys(:),us(:,:,plots(p))')
  axis equal, view(0,90)
  caxis(uRange), colormap(cMap), colorbar
  xlabel('space $x$'), ylabel('space $y$'), zlabel('$u(x,y,t)$')
  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 microstrucre has decayed leaving some random marginal modes starting to grow.

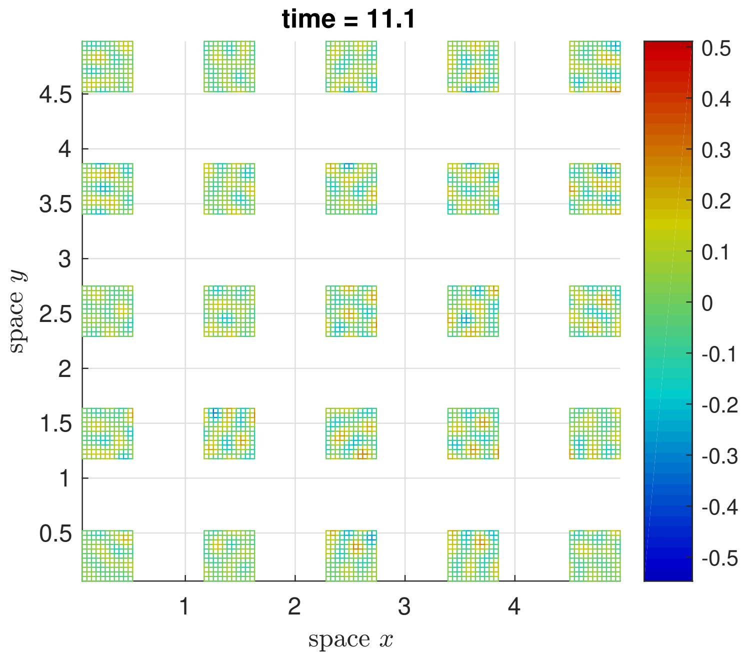
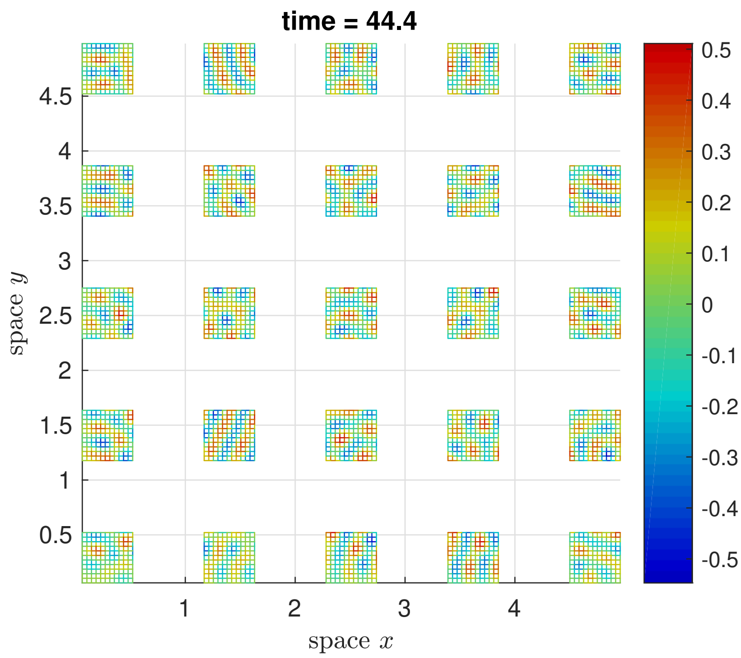


Figure 4.13: pattern field $u(x,y,t)$ in the patch scheme applied to a microscale discretisation of the 2D Swift–Hohenberg PDE. By now the local sub-patch patterns have reached a quasi-equilibrium amplitude.



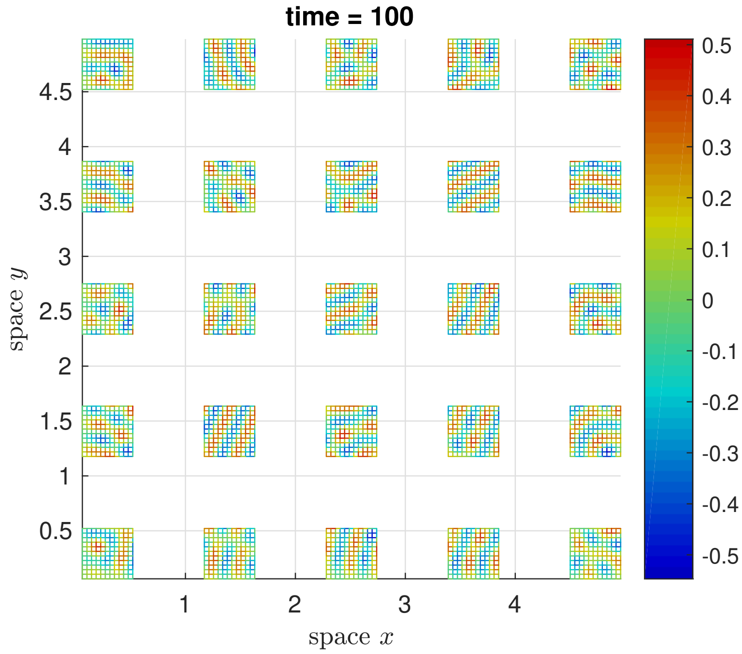


Figure 4.14: pattern field $u(x, y, t)$ in the patch scheme applied to a microscale discretisation of the 2D Swift–Hohenberg PDE. Patterns within the patches are evolving to the preferred rolls, but with weak coupling to other patches.

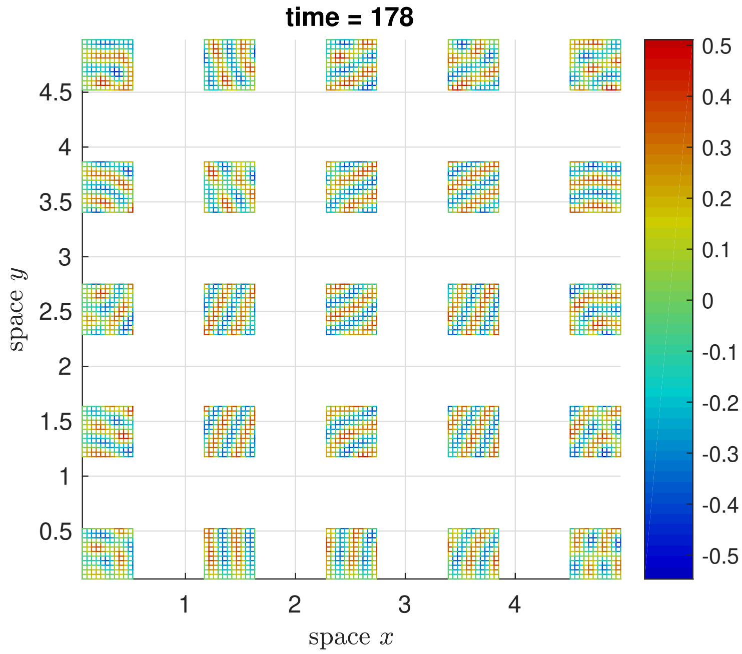


Figure 4.15: pattern field $u(x, y, t)$ in the patch scheme applied to a microscale discretisation of the 2D Swift–Hohenberg PDE. Can see different effects arising at different types of boundaries.

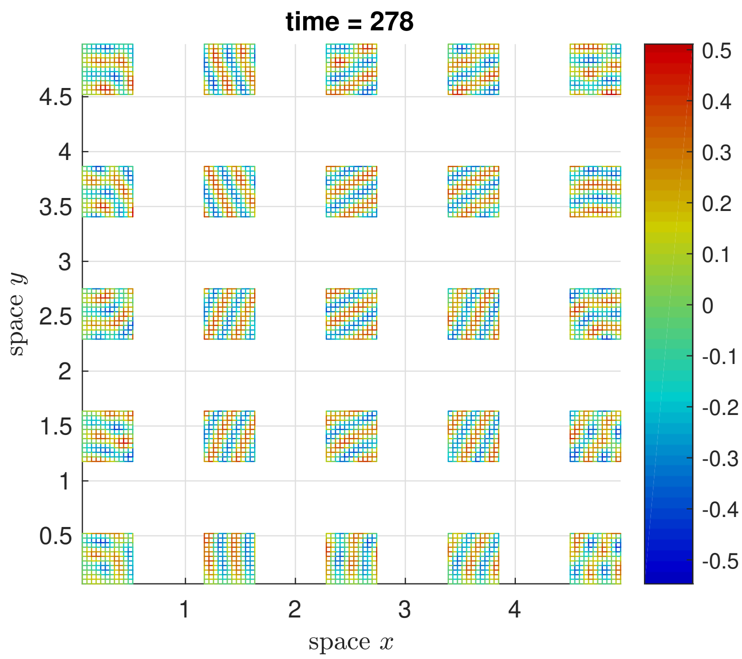


Figure 4.16: pattern field $u(x, y, t)$ in the patch scheme applied to a microscale discretisation of the 2D Swift–Hohenberg PDE. ...

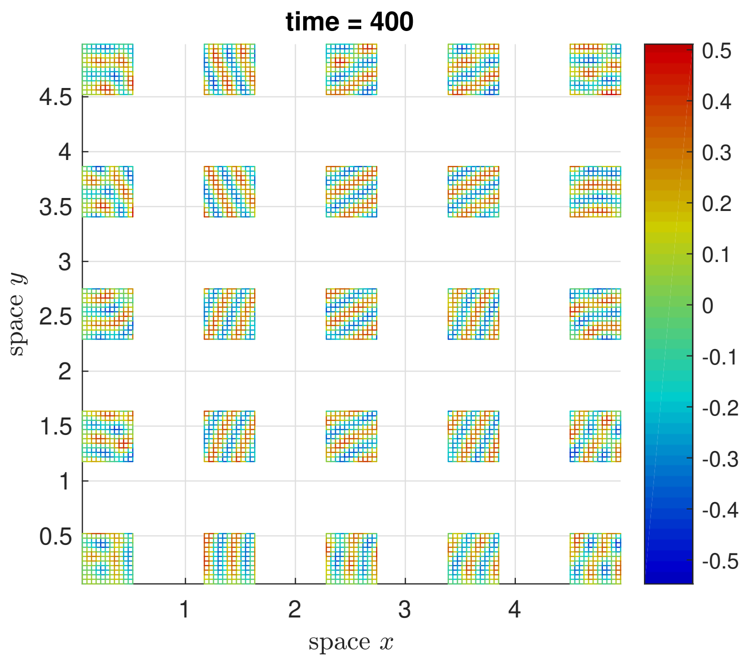


Figure 4.17: pattern field $u(x, y, t)$ in the patch scheme applied to a microscale discretisation of the 2D Swift–Hohenberg PDE. ...

```
  ifOurCf2eps([basename num2str(p)],[12 11])
end%for p
```

Third, plot animation in time: starts after a key press.

```
%%
figure(1),clf
cf=mesh(xs(:),ys(:),us(:,:,1)');
axis equal, view(0,90)
caxis(uRange), colormap(cMap), colorbar
xlabel('space $x$'), ylabel('space $y$'), zlabel('$u(x,y,t)$')
title(['time = ' num2str(ts(1),3)])
ca=gca;
disp('Press any key to start animation'),pause
for p=2:numel(ts)
  cf.ZData=us(:,:,p)';
  cf.CData=us(:,:,p)';
  ca.Title.String=['time = ' num2str(ts(p),3)];
  pause(0.1)
end
```

Fin.

4.13.1 The Swift–Hohenberg PDE and BCs inside patches

As a microscale discretisation of Swift–Hohenberg PDE $u_t = -(1+\nabla^2/k_0^2)^2u + \text{Ra}\,u - u^3$, here code straightforward centred discretisation in space.

```
function ut=SwiftHohenbergPDE(t,u,patches,k0,Ra)
  dx=diff(patches.x(1:2));  % microscale spacing
  dy=diff(patches.y(1:2));  % microscale spacing
  i=3:size(u,1)-2;  % interior points in patches
  j=3:size(u,2)-2;  % interior points in patches
```

Code various boundary conditions. For slightly simpler coding, squeeze out the two singleton dimensions.

```
  u = squeeze(u);
  u(1:2,:,1,:)=0; % u=u_x=0 at x=0
  u(:,1:2,:,1)=0; % u=u_y=0 at y=0
  u(end-1,:,end,:)=0;                 % u=0   at x=L
  u(end  ,:,end,:)=-u(end-2,:,end,:); % u_x=0 at x=L
  u(:,end-1,:,end)=-u(:,end-2,:,end); % u_y=0   at y=L
  u(:,end  ,:,end)=-u(:,end-3,:,end); % u_yyy=0 at y=L
```

Here code straightforward centred discretisation in space.

```
  ut=nan+u;         % preallocate output array
  v = u(2:end-1,2:end-1,:,:) ...
      +( diff(u(:,2:end-1,:,:),2,1)/dx^2 ...
        +diff(u(2:end-1,:,:,:),2,2)/dy^2 )/k0^2;
  ut(i,j,:,:) = -( v(2:end-1,2:end-1,:,:) ...
      +( diff(v(:,2:end-1,:,:),2,1)/dx^2 ...
```

```
        +diff(v(2:end-1,:,:,:),2,2)/dy^2 )/k0^2 ) ...
    +Ra*u(i,j,:,:) -u(i,j,:,:).^3;
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.

```
clear all, close all
global patches
nRealise = 20
```

4.13.2.1 Check divided difference interpolation

```
fprintf('\n\n**** Check divided difference interpolation\n')
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.)

```
maxErrors=[];
for realisation = 1:nRealise
    nEdge = randi(3,1,2)% =1,2, or 3
    edgyInt = (rand>0.5)
    Lx = 1+3*rand; Ly = 1+3*rand;
    xyLim = [0 Lx 0 Ly]-[rand*[1 1] rand*[1 1]]
    nSubP = nEdge.*( (2-edgyInt)*randi(3,1,2)+1+edgyInt )
    ordCC = 2*randi(4)
    nPatch = ordCC+randi(4,1,2)
    dx = [Lx Ly]./nPatch./nSubP.*rand(1,2)/2
    configPatches2(@sin,xyLim,'equispace',nPatch,ordCC ...
        ,dx,nSubP,'EdgyInt',edgyInt,'nEdge',nEdge);
```

Second, displace patches to a random non-uniform spacing.

```
Hx = diff(patches.x(1,1,:,:,1:2,1));
patches.x = patches.x+0.8*Hx*(rand(1,1,1,1,nPatch(1),1)-0.5);
Hx = squeeze( diff(patches.x(1,1,:,:,:,1)) );% for information only
Hy = diff(patches.y(1,1,:,:,:,1:2));
patches.y = patches.y+0.8*Hy*(rand(1,1,1,1,1,nPatch(2))-0.5);
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.

```
    ox=min(ordCC,nPatch(1)-1);
    oy=min(ordCC,nPatch(2)-1);
    [ps,qs]=ndgrid(0:ox,0:oy);
    ps=reshape(ps,1,1,[]);
    qs=reshape(qs,1,1,[]);
    cs=2*rand(size(ps))-1;
    u0=cs.*patches.x.^ps.*patches.y.^qs;
```

Then evaluate the interpolation, setting edges to `inf` for error checking.

```
    u=u0;
    u([1:nEdge(1)  end-nEdge(1)+1:end],:,:)=inf;
    u(:,[1:nEdge(2)  end-nEdge(2)+1:end],:)=inf;
    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.

```
    error = ui-u0;
    hist(log10(abs(error(abs(error)>1e-20))),-20:-7)
    xlabel('log10 error'), pause(0.3)%??
    maxError=max(abs(error(:)))
    maxErrors=[maxErrors maxError];
    assert(maxError<3e-12*4^ordCC ...
    ,'failed divided difference interpolation')
    disp('*** This divided difference test passed')
```

End the for-loops over various parameters.

```
end% for realisation
maxMaxErrorDividedDiffs = max(maxErrors)
disp('***** Passed all divided difference interpolation')
pause(1)
```

4.13.2.2 Test standard spectral interpolation

```
fprintf('\n\n**** Test standard spectral interpolation\n')
pause(1)
```

Test over various numbers of patches, random domain lengths and random ratios. Try realisations of random tests.

```
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.

```
nEdge=randi(3,1,2)% =1,2, or 3
edgyInt = (rand>0.5)
Lx = 1+3*rand, Ly = 1+3*rand
xyLim = [0 Lx 0 Ly]-[rand*[1 1] rand*[1 1]]
nSubP = nEdge.*( (2-edgyInt)*randi(3,1,2)+1+edgyInt )
nPatch = randi([3 6],1,2)
dx = [Lx Ly]./nPatch./nSubP.*rand(1,2)/2
configPatches2(@sin,xyLim,'periodic',nPatch,0 ...
    ,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.

```
nV=randi(3)
[nx,Nx]=size(squeeze(patches.x));
[ny,Ny]=size(squeeze(patches.y));
u0=nan(nx,ny,nV,1,Nx,Ny);
for iV=1:nV
  kx=randi([0 floor((nPatch(1)-1)/2)])
  ky=randi([0 floor((nPatch(2)-1)/2)])
  phix=pi*rand*(2*kx~=nPatch(1))
  phiy=pi*rand*(2*ky~=nPatch(2))
  % generate 6D array via auto-replication
  u0(:,:,iV,1,:,:)=sin(2*pi*kx*patches.x/Lx+phix) ...
                 .*sin(2*pi*ky*patches.y/Ly+phiy);
end
```

Copy and `nan` the edges, then interpolate

```
u=u0;
u([1:nEdge(1)  end-nEdge(1)+1:end],:,:)=nan;
u(:,[1:nEdge(2)  end-nEdge(2)+1:end],:)=nan;
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.

```
error = u-u0;
assert(all(~isnan(error(:))),'found nans in the error!')
hist(log10(abs(error(abs(error)>1e-20))),-20:-7)
xlabel('log10 error'), pause(0.3)%??
normError=norm(error(:))
assert(normError<1e-12, '2D spectral interpolation failed')
disp('*** This spectral test passed')
```

End the for-loop over realisations

```
end
disp('***** All the spectral tests passed')
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.)

```
for realisations=1:nRealise
    nEdge = randi(3,1,2)% =1,2, or 3
    edgyInt = (rand>0.5)
    nSubP = nEdge.*( (2-edgyInt)*randi(3,1,2)+1+edgyInt )
    ordCC = 2*randi(4)
    nPatch = ordCC+randi(4,1,2)
    xyLim=5*[-rand(1,2); rand(1,2)]
    dx = diff(xyLim)./nPatch./nSubP.*rand(1,2)/2
    configPatches2(@sin,xyLim,'periodic',nPatch,ordCC ...
        ,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.

```
    [ps,qs]=meshgrid(0:ordCC);
    ps=reshape(ps,1,1,[]); qs=reshape(qs,1,1,[]);
    cs=2*rand(size(ps))-1;
    u0=cs.*patches.x.^ps.*patches.y.^qs;
```

Then evaluate the interpolation.

```
    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.

```
    I=ordCC/2+1:nPatch(1)-ordCC/2;
    J=ordCC/2+1:nPatch(2)-ordCC/2;
    error=ui(:,:,:,:,I,J)-u0(:,:,:,:,I,J);
    assert(all(~isnan(error(:))),'found nans in the error!')
    hist(log10(abs(error(abs(error)>1e-20))),-20:-7)
    xlabel('log10 error'), pause(0.3)%??
    normError=norm(error(:))
    assert(normError<5e-9 ...
    ,'failed finite stencil interpolation')
    disp('*** This finite stencil test passed')
```

End the for-loops over various parameters.

```
end %for realisations
disp('***** Passed all standard polynomial interpolation')
```

4.13.2.4 Finished

If no error messages, then all OK.

```
disp('******* All the interpolation tests successful')
```

5 Patches in 3D space

5.1 `configPatches3()`: configures spatial patches in 3D

Section contents

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.

```
function patches = configPatches3(fun,Xlim,Dom ...
    ,nPatch,ordCC,dx,nSubP,varargin)
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)`] × [`Xlim(3)`, `Xlim(4)` × [`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 $0, 2, 4, \ldots$; 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` $= \frac{1}{2}$ 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 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` $:= m_x \cdot m_y \cdot m_z$ and construct an ensemble of all $m_x \cdot m_y \cdot m_z$ 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]

```
if nargout==0, global patches, end
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` $\times$ 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)` $\times 1 \times 1 \times 1 \times 1 \times$ `nPatch(1)` $\times 1 \times 1$ array of the regular spatial locations x_{iI} of the microscale grid points in every patch.
- `.y` (8D) is $1 \times$ `nSubP(2)` $\times 1 \times 1 \times 1 \times 1 \times$ `nPatch(2)` $\times 1$ array of the regular spatial locations y_{jJ} of the microscale grid points in every patch.
- `.z` (8D) is $1 \times 1 \times$ `nSubP(3)` $\times 1 \times 1 \times 1 \times 1 \times$ `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

```
if nargin==0
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.

```
mPeriod = [2 2 2];
cHetr = exp(0.9*randn([mPeriod 3]));
cHetr = cHetr*mean(1./cHetr(:))
```

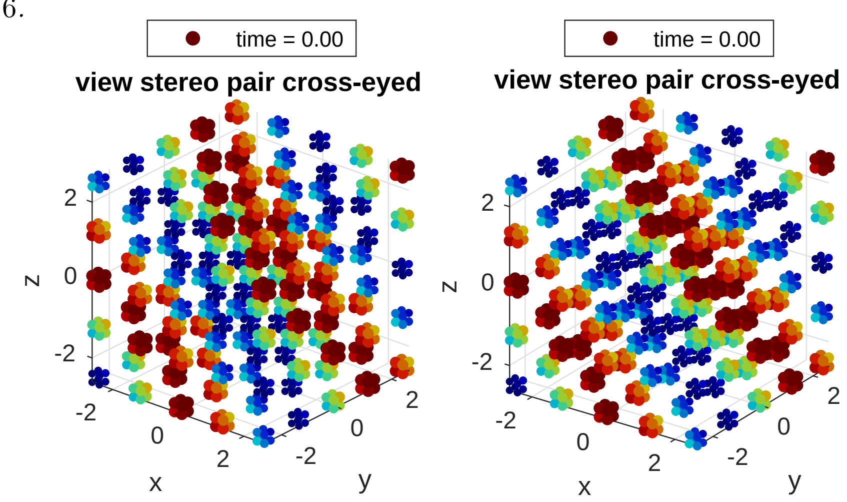
Establish global patch data struct to interface with a function coding a nonlinear 'diffusion' PDE: to be solved on $[-\pi,\pi]^3$-periodic domain, with 5^3 patches, spectral interpolation (0) couples the patches, each patch with micro-grid spacing 0.22 (relatively large for visualisation), and with 4^3 points forming each patch.

```
global patches
patches = configPatches3(@heteroWave3,[-pi pi] ...
    ,'periodic' , 5, 0, 0.22, mPeriod+2 ,'EdgyInt',true ...
    ,'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.

```
u0 = 0.5+0.5*sin(patches.x+patches.y+patches.z);
v0 =    -0.5*cos(patches.x+patches.y+patches.z)*sqrt(3);
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).

```
disp('Simulate heterogeneous wave u_tt=div[C*grad(u)]')
if ~exist('OCTAVE_VERSION','builtin')
    [ts,us] = ode23(@patchSys3,linspace(0,6),uv0(:));
else %disp('octave version is very slow for me')
    lsode_options('absolute tolerance',1e-4);
    lsode_options('relative tolerance',1e-4);
    [ts,us] = odeOcts(@patchSys3,[0 1 2],uv0(:));
end
```

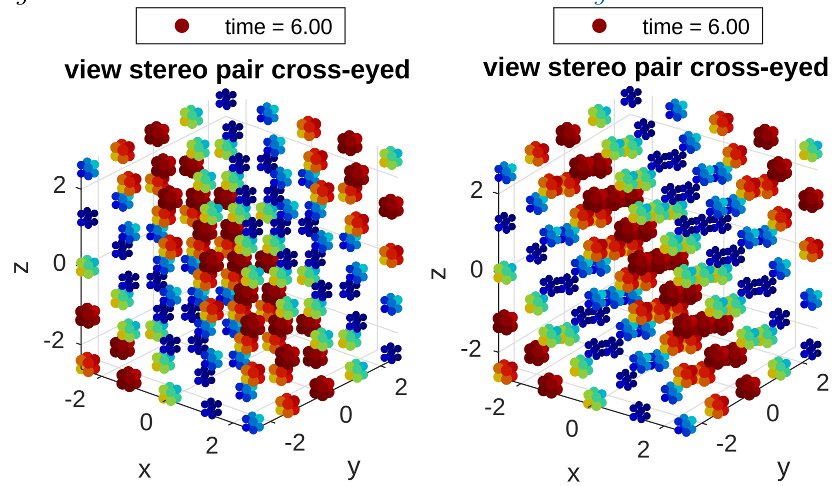
Animate the computed simulation to end with Figure 5.2. Use `patchEdgeInt3` to obtain patch-face values in order to most easily reconstruct the array data structure.

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.

```
figure(1), clf, colormap(0.8*jet)
xs = patches.x+0*patches.y+0*patches.z;
ys = patches.y+0*patches.x+0*patches.z;
zs = patches.z+0*patches.y+0*patches.x;
if 1, xs([1 end],:,:,:)=nan;
      xs(:,[1 end],:,:)=nan;
      xs(:,:,[1 end],:)=nan;
end;%option
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.




```
pix = @(u) 15*abs(u)+7;
col = @(u) sign(u).*abs(u);
```

Loop to plot at each and every time step.

```
for i = 1:length(ts)
  uv = patchEdgeInt3(us(i,:));
  u = uv(:,:,:,1,:);
  for p=1:2
    subplot(1,2,p)
    if (i==1)| exist('OCTAVE_VERSION','builtin')
      scat(p) = scatter3(xs(j),ys(j),zs(j),'filled');
      axis equal, caxis(col([0 1])), view(45-5*p,25)
      xlabel('$x$'), ylabel('$y$'), zlabel('$z$')
      title('view stereo pair cross-eyed')
    end % in matlab just update values
    set(scat(p),'CData',col(u(j)) ...
       ,'SizeData',pix((8+xs(j)-ys(j)+zs(j))/6+0*u(j)));
    legend(['time = ' num2str(ts(i),'%4.2f')],'Location','north')
  end
```

Optionally save the initial condition to graphic file for Figure 4.1, and optionally save the last plot.

```
  if i==1,
    ifOurCf2eps([mfilename 'ic'])
    disp('Type space character to animate simulation')
    pause
  else pause(0.05)
  end
end% i-loop over all times
ifOurCf2eps([mfilename 'fin'])
```

Upon finishing execution of the example, exit this function.

```
return
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^x_{ijk}, c^y_{ijk} and c^z_{ijk}, 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.

```
function ut = heteroWave3(t,u,patches)
  if nargin<3, global patches, end
```

Microscale space-steps, and interior point indices.

```
  dx = diff(patches.x(2:3));  % x micro-scale step
  dy = diff(patches.y(2:3));  % y micro-scale step
  dz = diff(patches.z(2:3));  % z micro-scale step
  i = 2:size(u,1)-1; % x interior points in a patch
  j = 2:size(u,2)-1; % y interior points in a patch
  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)`

```
  ut = nan+u;  % preallocate output array
  ut(i,j,k,1,:) = u(i,j,k,2,:);
  ut(i,j,k,2,:) ...
  =diff(patches.cs(:,j,k,1,:).*diff(u(:,j,k,1,:),1),1)/dx^2 ...
  +diff(patches.cs(i,:,k,2,:).*diff(u(i,:,k,1,:),1,2),1,2)/dy^2 ...
  +diff(patches.cs(i,j,:,3,:).*diff(u(i,j,:,1,:),1,3),1,3)/dz^2;
end% function
```

5.1.3 Parse input arguments and defaults

```
p = inputParser;
fnValidation = @(f) isa(f, 'function_handle'); %test for fn name
addRequired(p,'fun',fnValidation);
addRequired(p,'Xlim',@isnumeric);
%addRequired(p,'Dom'); % too flexible
addRequired(p,'nPatch',@isnumeric);
addRequired(p,'ordCC',@isnumeric);
addRequired(p,'dx',@isnumeric);
addRequired(p,'nSubP',@isnumeric);
addParameter(p,'nEdge',1,@isnumeric);
```

```
addParameter(p,'EdgyInt',false,@islogical);
addParameter(p,'nEnsem',1,@isnumeric);
addParameter(p,'hetCoeffs',[],@isnumeric);
addParameter(p,'parallel',false,@islogical);
%addParameter(p,'nCore',1,@isnumeric); % not yet implemented
parse(p,fun,Xlim,nPatch,ordCC,dx,nSubP,varargin{:});
```

Set the optional parameters.

```
patches.nEdge = p.Results.nEdge;
if numel(patches.nEdge)==1
    patches.nEdge = repmat(patches.nEdge,1,3);
    end
patches.EdgyInt = p.Results.EdgyInt;
patches.nEnsem = p.Results.nEnsem;
cs = p.Results.hetCoeffs;
patches.parallel = p.Results.parallel;
%patches.nCore = p.Results.nCore;
```

Initially duplicate parameters for three space dimensions as needed.

```
if numel(Xlim)==2,   Xlim = repmat(Xlim,1,3); end
if numel(nPatch)==1, nPatch = repmat(nPatch,1,3); end
if numel(dx)==1,     dx = repmat(dx,1,3); end
if numel(nSubP)==1,  nSubP = repmat(nSubP,1,3); end
```

Check parameters.

```
assert(Xlim(1)<Xlim(2) ...
      ,'first pair of Xlim must be ordered increasing')
assert(Xlim(3)<Xlim(4) ...
      ,'second pair of Xlim must be ordered increasing')
assert(Xlim(5)<Xlim(6) ...
      ,'third pair of Xlim must be ordered increasing')
assert((mod(ordCC,2)==0)|all(patches.nEdge==1) ...
      ,'Cannot yet have nEdge>1 and staggered patch grids')
assert(all(3*patches.nEdge<=nSubP) ...
      ,'too many edge values requested')
assert(all(rem(nSubP,patches.nEdge)==0) ...
      ,'nSubP must be integer multiple of nEdge')
if ~patches.EdgyInt, assert(all(rem(nSubP./patches.nEdge,2)==1) ...
      ,'for non-edgyInt, nSubP./nEdge must be odd integer')
      end
if (patches.nEnsem>1)&all(patches.nEdge>1)
      warning('not yet tested when both nEnsem and nEdge non-one')
      end
%if patches.nCore>1
%    warning('nCore>1 not yet tested in this version')
%    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.

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

Default macroscale conditions are periodic with evenly spaced patches.

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

```
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.

```
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 boundaries if no `bcOffset` specified when needed. Do so for all three directions independently.

```
patches.periodic=false;
for p=1:3
switch Dom.type(p,:)
case 'periodic'
    patches.periodic=true;
    if isfield(Dom,'bcOffset')
    warning('bcOffset not available for Dom.type = periodic'), end
    msg=' not available for Dom.type = periodic';
    if isfield(Dom,'X'), warning(['X' msg]), end
    if isfield(Dom,'Y'), warning(['Y' msg]), end
    if isfield(Dom,'Z'), warning(['Z' msg]), end
case {'equispace','chebyshev'}
    if ~isfield(Dom,'bcOffset'), Dom.bcOffset=zeros(2,3); end
    % for mixed with usergiven, following should still work
    if numel(Dom.bcOffset)==1
        Dom.bcOffset=repmat(Dom.bcOffset,2,3); end
    if numel(Dom.bcOffset)==3
        Dom.bcOffset=repmat(Dom.bcOffset(:)',2,1); end
    msg=' not available for Dom.type = equispace or chebyshev';
    if (p==1)& isfield(Dom,'X'), warning(['X' msg]), end
    if (p==2)& isfield(Dom,'Y'), warning(['Y' msg]), end
    if (p==3)& isfield(Dom,'Z'), warning(['Z' msg]), end
case 'usergiven'
%    if isfield(Dom,'bcOffset')
%    warning('bcOffset not available for usergiven Dom.type'), end
    msg=' required for Dom.type = usergiven';
```

```
    if p==1, assert(isfield(Dom,'X'),['X' msg]), end
    if p==2, assert(isfield(Dom,'Y'),['Y' msg]), end
    if p==3, assert(isfield(Dom,'Z'),['Z' msg]), end
otherwise
    error([Dom.type ' is unknown Dom.type'])
end%switch Dom.type
end%for p
```

5.1.4 The code to make patches

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

```
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.

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

For odd `ordCC` do interpolation based upon odd neighbouring patches as is useful for staggered grids.

```
patches.stag = mod(ordCC,2);
assert(patches.stag==0,'staggered not yet implemented??')
ordCC = ordCC+patches.stag;
patches.ordCC = ordCC;
```

Check for staggered grid and periodic case.

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

```
for q=1:3
qq=2*q-1;
```

Distribution depends upon `Dom.type`:

```
switch Dom.type(q,:)
```

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

```
case 'periodic'
  Q=linspace(Xlim(qq),Xlim(qq+1),nPatch(q)+1);
  DQ=Q(2)-Q(1);
  Q=Q(1:nPatch(q))+diff(Q)/2;
  pEI=patches.EdgyInt;% abbreviation
```

```
  pnE=patches.nEdge(q);% abbreviation
  if pre2023, dx(q) = ratio(q)*DQ/(nSubP(q)-pnE*(1+pEI))*(2-pEI);
  else        ratio(q) = dx(q)/DQ*(nSubP(q)-pnE*(1+pEI))/(2-pEI);
  end
  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.

```
case 'equispace'
  Q=linspace(Xlim(qq)+((nSubP(q)-1)/2-Dom.bcOffset(qq))*dx(q) ...
          ,Xlim(qq+1)-((nSubP(q)-1)/2-Dom.bcOffset(qq+1))*dx(q) ...
          ,nPatch(q));
  DQ=diff(Q(1:2));
  width=(1+patches.EdgyInt)/2*(nSubP(q)-1-patches.EdgyInt)*dx;
  if DQ<width*0.999999
     warning('too many equispace patches (double overlapping)')
     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]

```
case 'chebyshev'
  halfWidth=dx(q)*(nSubP(q)-1)/2;
  Q1 = Xlim(1)+halfWidth-Dom.bcOffset(qq)*dx(q);
  Q2 = Xlim(2)-halfWidth+Dom.bcOffset(qq+1)*dx(q);
%  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`.

```
  pEI=patches.EdgyInt; % abbreviation
  pnE=patches.nEdge(q);% abbreviation
  width=(1+pEI)/2*(nSubP(q)-pnE*(1+pEI))*dx(q);
  for b=0:2:nPatch(q)-2
    DQmin=(Q2-Q1-b*width)/2*( 1-cos(pi/(nPatch(q)-b-1)) );
    if DQmin>width, break, end
  end%for
  if DQmin<width*0.999999
    warning('too many Chebyshev patches (mid-domain overlap)')
  end%if
```

Assign the centre-patch coordinates.

```
  Q =[ Q1+(0:b/2-1)*width ...
       (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??

```
        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.

```
case 'usergiven'
  if q==1, Q = reshape(Dom.X,1,[]); end
  if q==2, Q = reshape(Dom.Y,1,[]); end
  if q==3, Q = reshape(Dom.Z,1,[]); end
end%switch Dom.type
```

Assign Q-coordinates to the correct spatial direction. At this stage they are all rows.

```
if q==1, X=Q; end
if q==2, Y=Q; end
if q==3, Z=Q; end
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).

```
xs = dx(1)*( (1:nSubP(1))-mean(1:nSubP(1)) );
patches.x = reshape( xs'+X ...
                   ,nSubP(1),1,1,1,1,nPatch(1),1,1);
ys = dx(2)*( (1:nSubP(2))-mean(1:nSubP(2)) );
patches.y = reshape( ys'+Y ...
                   ,1,nSubP(2),1,1,1,1,nPatch(2),1);
zs = dx(3)*( (1:nSubP(3))-mean(1:nSubP(3)) );
patches.z = reshape( zs'+Z ...
                   ,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]

```
if patches.periodic
  ratio = reshape(ratio,1,3); % force to be row vector
  patches.ratio = ratio;
  if ordCC>0
      [Cwtsr,Cwtsl] = patchCwts(ratio,ordCC,patches.stag);
      patches.Cwtsr = Cwtsr;  patches.Cwtsl = Cwtsl;
  end%if
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()`.

```
nE = patches.nEnsem;
patches.le = 1:nE;  patches.ri = 1:nE;
patches.bo = 1:nE;  patches.to = 1:nE;
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 then 4D, then the higher-dimensions are reshaped into the 4th dimension.

```
if ~isempty(cs)
  [mx,my,mz,nc] = size(cs);
  nx = nSubP(1); ny = nSubP(2); nz = nSubP(3);
  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.

```
  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.

```
    patches.nEnsem = mx*my*mz;
    patches.cs = nan(nx-1,ny-1,nz-1,nc,mx,my,mz);
    for k = 1:mz
      ks = (k:k+nz-2);
      for j = 1:my
        js = (j:j+ny-2);
        for i = 1:mx
          is = (i:i+nx-2);
          patches.cs(:,:,:,:,i,j,k) = cs(is,js,ks,:);
        end
      end
    end
    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.

```
    mmx=(0:mx-1)’; mmy=0:my-1; mmz=shiftdim(0:mz-1,-1);
    le = mod(mmx+mod(nx-2,mx),mx)+1;
    patches.le = reshape(  le+mx*(mmy+my*mmz)  ,[],1);
    ri = mod(mmx-mod(nx-2,mx),mx)+1;
    patches.ri = reshape(  ri+mx*(mmy+my*mmz)  ,[],1);
    bo = mod(mmy+mod(ny-2,my),my)+1;
    patches.bo = reshape( 1+mmx+mx*(bo-1+my*mmz) ,[],1);
    to = mod(mmy-mod(ny-2,my),my)+1;
    patches.to = reshape( 1+mmx+mx*(to-1+my*mmz) ,[],1);
    ba = mod(mmz+mod(nz-2,mz),mz)+1;
    patches.ba = reshape( 1+mmx+mx*(mmy+my*(ba-1)) ,[],1);
    fr = mod(mmz-mod(nz-2,mz),mz)+1;
    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]

```
if prod(ratio)*patches.nEnsem>0.9, warning( ...
’Probably poor scale separation in ensemble of coupled phase-shifts’)
scaleSeparationParameter = ratio*patches.nEnsem
end
```

End the two if-statements.

```
  end%if-else nEnsem>1
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]

```
if patches.parallel
  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.

```
  [~,pari]=max(nPatch+0.01*(1:3));
  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’)`.

```
  switch pari
    case 1, patches.x=codistributed(patches.x,patches.codist);
    case 2, patches.y=codistributed(patches.y,patches.codist);
    case 3, patches.z=codistributed(patches.z,patches.codist);
  otherwise
    error('should never have bad index for parallel distribution')
  end%switch
  end%spmd
```

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

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

Fin

```
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.

```
function dudt = patchSys3(t,u,patches,varargin)
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)`×`nSubP(3)`×`nPatch(1)`×`nPatch(2)`×`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 `nSubP(1)`×`nSubP(2)`×`nSubP(3)`×`nVars`×`nEsem`× `nPatch(1)` × `nPatch(2)` × `nPatch(3)`. 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 × 1`nPatch(1)` × 1 × 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 × `nSubP(2)` × 1 × 1 × 1 × 1 × `nPatch(2)` × 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 × 1 × `nSubP(3)` × 1 × 1 × 1 × 1 × `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 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()`.

```
sizeu = size(u);
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.

```
dudt = patches.fun(t,u,patches,varargin{:});
m = patches.nEdge(1);
dudt([1:m end-m+1:end],:,:,:) = 0;
m = patches.nEdge(2);
dudt(:,[1:m end-m+1:end],:,:) = 0;
m = patches.nEdge(3);
dudt(:,:,[1:m end-m+1:end],:) = 0;
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`.

```
function u = patchEdgeInt3(u,patches)
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` · `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 `nSubP1` $\times 1\times 1\times 1\times 1\times$ `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 $1\times$ `nSubP2` $\times 1\times 1\times 1\times 1\times$ `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 $1\times 1\times$ `nSubP3` $\times 1\times 1\times 1\times 1\times$ `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 $\{0,2,4,\ldots\}$
  - `.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, `nSubP1` · `nSubP2` · `nSubP3` · `nVars` · `nEnsem` · `nPatch1` · `nPatch2` · `nPatch3`, 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.

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

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

```
[~,~,nz,~,~,~,~,Nz] = size(patches.z);
[~,ny,~,~,~,~,Ny,~] = size(patches.y);
[nx,~,~,~,~,Nx,~,~] = size(patches.x);
nEnsem = patches.nEnsem;
nVars = round( numel(u)/numel(patches.x) ...
    /numel(patches.y)/numel(patches.z)/nEnsem );
assert(numel(u) == nx*ny*nz*Nx*Ny*Nz*nVars*nEnsem ...
  ,'patchEdgeInt3: input u has wrong size for parameters')
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.

```
I=1:Nx; Ip=mod(I,Nx)+1; Im=mod(I-2,Nx)+1;
J=1:Ny; Jp=mod(J,Ny)+1; Jm=mod(J-2,Ny)+1;
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.

```
%x = patches.x;
%if patches.nEdge(1)>1
%  m = patches.nEdge(1);
%  x = x(1:m:nx,:,:,:,:,:,:,:);
%  nx = nx/m;
%  u = reshape(u,m,nx,ny,nz,nVars,nEnsem,Nx,Ny,Nz);
%  nVars = nVars*m;
%  u = reshape( permute(u,[2:4 1 5:9]) ...
%             ,nx,ny,nz,nVars,nEnsem,Nx,Ny,Nz);
%end%if patches.nEdge(1)
%y = patches.y;
%if patches.nEdge(2)>1
%  m = patches.nEdge(2);
%  y = y(:,1:m:ny,:,:,:,:,:,:);
%  ny = ny/m;
%  u = reshape(u,nx,m,ny,nz,nVars,nEnsem,Nx,Ny,Nz);
%  nVars = nVars*m;
%  u = reshape( permute(u,[1 3:4 2 5:9]) ...
%             ,nx,ny,nz,nVars,nEnsem,Nx,Ny,Nz);
%end%if patches.nEdge(2)
%z = patches.z;
%if patches.nEdge(3)>1
%  m = patches.nEdge(3);
%  z = z(:,:,1:m:nz,:,:,:,:,:);
%  nz = nz/m;
%  u = reshape(u,nx,ny,m,nz,nVars,nEnsem,Nx,Ny,Nz);
%  nVars = nVars*m;
%  u = reshape( permute(u,[1:2 4 3 5:9]) ...
%             ,nx,ny,nz,nVars,nEnsem,Nx,Ny,Nz);
%end%if patches.nEdge(3)
x = patches.x;
y = patches.y;
z = patches.z;
if mean(patches.nEdge)>1
  mx = patches.nEdge(1);
  my = patches.nEdge(2);
  mz = patches.nEdge(3);
  x = x(1:mx:nx,:,:,:,:,:,:,:);
  y = y(:,1:my:ny,:,:,:,:,:,:);
  z = z(:,:,1:mz:nz,:,:,:,:,:);
  nx = nx/mx;
  ny = ny/my;
  nz = nz/mz;
  u = reshape(u,mx,nx,my,ny,mz,nz,nVars,nEnsem,Nx,Ny,Nz);
  nVars = nVars*mx*my*mz;
```

```
  u = reshape( permute(u,[2:2:6 1:2:5 7:11]) ...
             ,nx,ny,nz,nVars,nEnsem,Nx,Ny,Nz);
end%if patches.nEdge
```

The centre of each patch (as `nx`, `ny` and `nz` are odd for centre-patch interpolation) is at indices

```
i0 = round((nx+1)/2);
j0 = round((ny+1)/2);
k0 = round((nz+1)/2);
```

5.3.1 Periodic macroscale interpolation schemes

```
if patches.periodic
```

Get the size ratios of the patches in each direction.

```
rx = patches.ratio(1);
ry = patches.ratio(2);
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.

```
ordCC = patches.ordCC;
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.

```
  if patches.EdgyInt % interpolate next-to-face values
    U = u([2 nx-1],2:(ny-1),2:(nz-1),:,:,I,J,K);
  else % interpolate centre-cross values
    U = u(i0,2:(ny-1),2:(nz-1),:,:,I,J,K);
  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.

```
szUO=size(U); szUO=[szUO ones(1,8-length(szUO)) ordCC];
```

Use finite difference formulas for the interpolation, so store finite differences $(\mu\delta, \delta^2, \mu\delta^3, \delta^4, \ldots)$ in these arrays. When parallel, in order to preserve the distributed array structure we use an index at the end for the differences.

```
  if ~patches.parallel, dmu = zeros(szUO); % 9D
  else   dmu = zeros(szUO,patches.codist); % 9D
  end%if patches.parallel
```

First compute differences $\mu\delta$ and δ^2.

```
  if patches.stag % use only odd numbered neighbours
    error('polynomial interpolation not yet for staggered patch coupling')
%     dmux(:,:,:,:,:,I,:,:,1) = (Ux(:,:,:,:,:,Ip,:,:) +Ux(:,:,:,:,:,Im,:,:))/2
%     dmux(:,:,:,:,:,I,:,:,2) = (Ux(:,:,:,:,:,Ip,:,:) -Ux(:,:,:,:,:,Im,:,:));
%     Ip = Ip(Ip); Im = Im(Im); % increase shifts to \pm2
%     dmuy(:,:,:,:,:,:,J,:,1) = (Ux(:,:,:,:,:,:,Jp,:)+Ux(:,:,:,:,:,:,Jm,:))/2;
%     dmuy(:,:,:,:,:,:,J,:,2) = (Ux(:,:,:,:,:,:,Jp,:)-Ux(:,:,:,:,:,:,Jm,:)); %
%     Jp = Jp(Jp); Jm = Jm(Jm); % increase shifts to \pm2
%     dmuz(:,:,:,:,:,:,:,K,1) = (Ux(:,:,:,:,:,:,:,Kp)+Ux(:,:,:,:,:,:,:,Km))/2;
%     dmuz(:,:,:,:,:,:,:,K,2) = (Ux(:,:,:,:,:,:,:,Kp)-Ux(:,:,:,:,:,:,:,Km)); %
%     Kp = Kp(Kp); Km = Km(Km); % increase shifts to \pm2
  else  %disp('starting standard interpolation')
    dmu(:,:,:,:,:,I,:,:,1) = (U(:,:,:,:,:,Ip,:,:) ...
                             -U(:,:,:,:,:,Im,:,:))/2; %\mu\delta
    dmu(:,:,:,:,:,I,:,:,2) = (U(:,:,:,:,:,Ip,:,:) ...
       -2*U(:,:,:,:,:,I,:,:) +U(:,:,:,:,:,Im,:,:));   %\delta^2
  end% if stag
```

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

```
  for k = 3:ordCC
    dmu(:,:,:,:,:,I,:,:,k) =     dmu(:,:,:,:,:,Ip,:,:,k-2) ...
    -2*dmu(:,:,:,:,:,I,:,:,k-2) +dmu(:,:,:,:,:,Im,:,:,k-2);
  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`.

```
k=1+patches.EdgyInt; % use centre or two faces
u(nx,2:(ny-1),2:(nz-1),:,patches.ri,I,:,:) ...
  = U(1,:,:,:,:,:,:,:)*(1-patches.stag) ...
  +sum( shiftdim(patches.Cwtsr(:,1),-8).*dmu(1,:,:,:,:,:,:,:,:) ,9);
u(1 ,2:(ny-1),2:(nz-1),:,patches.le,I,:,:) ...
  = U(k,:,:,:,:,:,:,:)*(1-patches.stag) ...
  +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.

```
  if patches.EdgyInt % interpolate next-to-face values
    U = u(:,[2 ny-1],2:(nz-1),:,:,I,J,K);
  else % interpolate centre-cross values
    U = u(:,j0,2:(nz-1),:,:,I,J,K);
  end;%if patches.EdgyInt
```

Adjoin extra dimension for the array of differences.

```
szUO=size(U); szUO=[szUO ones(1,8-length(szUO)) ordCC];
```

Store finite differences $(\mu\delta, \delta^2, \mu\delta^3, \delta^4, \ldots)$ in this array.

```
  if ~patches.parallel, dmu = zeros(szUO); % 9D
  else   dmu = zeros(szUO,patches.codist); % 9D
  end%if patches.parallel
```

First compute differences $\mu\delta$ and δ^2.

```
  if patches.stag % use only odd numbered neighbours
    error('polynomial interpolation not yet for staggered patch coupling')
  else  %disp('starting standard interpolation')
    dmu(:,:,:,:,:,:,J,:,1) = (U(:,:,:,:,:,:,Jp,:) ...
                             -U(:,:,:,:,:,:,Jm,:))/2; %\mu\delta
    dmu(:,:,:,:,:,:,J,:,2) = (U(:,:,:,:,:,:,Jp,:) ...
       -2*U(:,:,:,:,:,:,J,:) +U(:,:,:,:,:,:,Jm,:));   %\delta^2
  end% if stag
```

Recursively take δ^2.

```
  for k = 3:ordCC
    dmu(:,:,:,:,:,:,J,:,k) =     dmu(:,:,:,:,:,:,Jp,:,k-2) ...
    -2*dmu(:,:,:,:,:,:,J,:,k-2) +dmu(:,:,:,:,:,:,Jm,:,k-2);
  end
```

Interpolate macro-values using the weights pre-computed by `configPatches3()`. An ensemble of configurations may have cross-coupling.

```
k=1+patches.EdgyInt; % use centre or two faces
u(:,ny,2:(nz-1),:,patches.to,:,J,:) ...
  = U(:,1,:,:,:,:,:,:)*(1-patches.stag) ...
  +sum( shiftdim(patches.Cwtsr(:,2),-8).*dmu(:,1,:,:,:,:,:,:,:) ,9);
u(:,1 ,2:(nz-1),:,patches.bo,:,J,:) ...
  = U(:,k,:,:,:,:,:,:)*(1-patches.stag) ...
  +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.

```
  if patches.EdgyInt % interpolate next-to-face values
    U = u(:,:,[2 nz-1],:,:,I,J,K);
  else % interpolate centre-cross values
    U = u(:,:,k0,:,:,I,J,K);
  end;%if patches.EdgyInt
```

Adjoin extra dimension for the array of differences.

```
szUO=size(U); szUO=[szUO ones(1,8-length(szUO)) ordCC];
```

Store finite differences ($\mu\delta, \delta^2, \mu\delta^3, \delta^4, \ldots$) in this array.

```
  if ~patches.parallel, dmu = zeros(szUO); % 9D
  else   dmu = zeros(szUO,patches.codist); % 9D
  end%if patches.parallel
```

First compute differences $\mu\delta$ and δ^2.

```
  if patches.stag % use only odd numbered neighbours
    error('polynomial interpolation not yet for staggered patch coupling')
  else  %disp('starting standard interpolation')
    dmu(:,:,:,:,:,:,:,K,1) = (U(:,:,:,:,:,:,:,Kp) ...
                             -U(:,:,:,:,:,:,:,Km))/2; %\mu\delta
    dmu(:,:,:,:,:,:,:,K,2) = (U(:,:,:,:,:,:,:,Kp) ...
       -2*U(:,:,:,:,:,:,:,K) +U(:,:,:,:,:,:,:,Km));   %\delta^2
  end% if stag
```

Recursively take δ^2.

```
  for k = 3:ordCC
    dmu(:,:,:,:,:,:,:,K,k) =     dmu(:,:,:,:,:,:,:,Kp,k-2) ...
    -2*dmu(:,:,:,:,:,:,:,K,k-2) +dmu(:,:,:,:,:,:,:,Km,k-2);
  end
```

Interpolate macro-values using the weights pre-computed by `configPatches3()`. An ensemble of configurations may have cross-coupling.

```
k=1+patches.EdgyInt; % use centre or two faces
u(:,:,nz,:,patches.fr,:,:,K) ...
  = U(:,:,1,:,:,:,:,:)*(1-patches.stag) ...
  +sum( shiftdim(patches.Cwtsr(:,3),-8).*dmu(:,:,1,:,:,:,:,:,:) ,9);
u(:,:,1 ,:,patches.ba,:,:,K) ...
  = U(:,:,k,:,:,:,:,:)*(1-patches.stag) ...
  +sum( shiftdim(patches.Cwtsl(:,3),-8).*dmu(:,:,k,:,:,:,:,:,:) ,9);
```

5.3.1.2 Case of spectral interpolation

Assumes the domain is macro-periodic.

```
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 $\texttt{ks} = k2\pi/N$ for 'wavenumbers' $k = (0, 1, \ldots, k_{\max}, -k_{\max}, \ldots, -1)$ for odd N, and $k = (0, 1, \ldots, k_{\max}, \pm(k_{\max}+1) - k_{\max}, \ldots, -1)$ 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.

```
 if patches.stag % transform by doubling the number of fields
 error('staggered grid not yet implemented??')
   v=nan(size(u)); % currently to restore the shape of u
   u=cat(3,u(:,1:2:nPatch,:),u(:,2:2:nPatch,:));
   stagShift=reshape(0.5*[ones(nVars,1);-ones(nVars,1)],1,1,[]);
   iV=[nVars+1:2*nVars 1:nVars]; % scatter interp to alternate field
   r=r/2;           % ratio effectively halved
   nPatch=nPatch/2; % halve the number of patches
   nVars=nVars*2;   % double the number of fields
 else % the values for standard spectral
    stagShift = 0;
    iV = 1:nVars;
 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.

```
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, $k = (0\,, 1\,, \ldots, k_{\max}\,, +(k_{\max}+1) - k_{\max}\,, \ldots, -1)$.

```
  kMax = floor((Nx-1)/2);
  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`.

```
if ~patches.EdgyInt
     Cm = fft( u(i0,iy,iz,:,:,:,:,:) ,[],6);
     Cp = Cm;
else
     Cm = fft( u(   2,iy,iz ,:,patches.le,:,:,:) ,[],6);
     Cp = fft( u(nx-1,iy,iz ,:,patches.ri,:,:,:) ,[],6);
end%if ~patches.EdgyInt
```

Now invert the Fourier transforms to complete interpolation. Enforce reality when appropriate.

```
u(nx,iy,iz,:,:,:,:,:) = uclean( ifft( ...
    Cm.*exp(1i*(stagShift+kr))  ,[],6) );
```

```
u( 1,iy,iz,:,:,:,:,:) = uclean( ifft( ...
    Cp.*exp(1i*(stagShift-kr))  ,[],6) );
```

y-normal face values Set wavenumbers into a vector.

```
  kMax = floor((Ny-1)/2);
  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.

```
if ~patches.EdgyInt
     Cm = fft( u(:,j0,iz,:,:,:,:,:) ,[],7);
     Cp = Cm;
else
     Cm = fft( u(:,2   ,iz ,:,patches.bo,:,:,:) ,[],7);
     Cp = fft( u(:,ny-1,iz ,:,patches.to,:,:,:) ,[],7);
end%if ~patches.EdgyInt
```

Invert the Fourier transforms to complete interpolation.

```
u(:,ny,iz,:,:,:,:,:) = uclean( ifft( ...
    Cm.*exp(1i*(stagShift+kr))  ,[],7) );
u(:, 1,iz,:,:,:,:,:) = uclean( ifft( ...
    Cp.*exp(1i*(stagShift-kr))  ,[],7) );
```

z-normal face values Set wavenumbers into a vector.

```
  kMax = floor((Nz-1)/2);
  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.

```
if ~patches.EdgyInt
     Cm = fft( u(:,:,k0,:,:,:,:,:) ,[],8);
     Cp = Cm;
else
     Cm = fft( u(:,:,2    ,:,patches.ba,:,:,:) ,[],8);
     Cp = fft( u(:,:,nz-1 ,:,patches.fr,:,:,:) ,[],8);
end%if ~patches.EdgyInt
```

Invert the Fourier transforms to complete interpolation.

```
u(:,:,nz,:,:,:,:,:) = uclean( ifft( ...
    Cm.*exp(1i*(stagShift+kr))  ,[],8) );
u(:,:, 1,:,:,:,:,:) = uclean( ifft( ...
    Cp.*exp(1i*(stagShift-kr))  ,[],8) );
```

```
end% if ordCC>0
```

5.3.2 Non-periodic macroscale interpolation

```
else% patches.periodic false
assert(~patches.stag, ...
'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 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.

```
if patches.ordCC<1
     px = Nx-1;  py = Ny-1;  pz = Nz-1;
else px = min(patches.ordCC,Nx-1);
     py = min(patches.ordCC,Ny-1);
     pz = min(patches.ordCC,Nz-1);
end
% interior indices of faces  (ix n/a)
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]

```
  F = nan(patches.EdgyInt+1,ny-2,nz-2,nVars,nEnsem,Nx,Ny,Nz,px+1);
  if patches.EdgyInt % interpolate next-to-face values
    F(:,:,:,:,:,:,:,:,1) = u([nx-1 2],iy,iz,:,:,:,:,:);
    X = x([nx-1 2],:,:,:,:,:,:,:);
  else % interpolate mid-patch cross-patch values
    F(:,:,:,:,:,:,:,:,1) = u(i0,iy,iz,:,:,:,:,:);
    X = x(i0,:,:,:,:,:,:,:);
  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.

```
for q = 1:px
  i = 1:Nx-q;
  F(:,:,:,:,:,i,:,:,q+1) ...
  = ( F(:,:,:,:,:,i+1,:,:,q)-F(:,:,:,:,:,i,:,:,q)) ...
   ./(X(:,:,:,:,:,i+q,:,:)  -X(:,:,:,:,:,i,:,:));
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 `Xface` for every interior `Y,Z`.

```
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.

```
  i = max(1,min(1:Nx,Nx-ceil(px/2))-floor(px/2));
  Uface = F(:,:,:,:,:,i,:,:,px+1);
  for q = px:-1:1
    Uface = F(:,:,:,:,:,i,:,:,q) ...
    +(Xface-X(:,:,:,:,:,i+q-1,:,:)).*Uface;
  end
```

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

```
u(1 ,iy,iz,:,patches.le,:,:,:) = Uface(1,:,:,:,:,:,:,:);
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.

```
  F = nan(nx,patches.EdgyInt+1,nz-2,nVars,nEnsem,Nx,Ny,Nz,py+1);
  if patches.EdgyInt % interpolate next-to-face values
    F(:,:,:,:,:,:,:,:,1) = u(:,[ny-1 2],iz,:,:,:,:,:);
    Y = y(:,[ny-1 2],:,:,:,:,:,:);
  else % interpolate mid-patch cross-patch values
    F(:,:,:,:,:,:,:,:,1) = u(:,j0,iz,:,:,:,:,:);
    Y = y(:,j0,:,:,:,:,:,:);
  end%if patches.EdgyInt
```

Form tables of divided differences.

```
for q = 1:py
  j = 1:Ny-q;
  F(:,:,:,:,:,:,j,:,q+1) ...
  = ( F(:,:,:,:,:,:,j+1,:,q)-F(:,:,:,:,:,:,j,:,q)) ...
   ./(Y(:,:,:,:,:,:,j+q,:)  -Y(:,:,:,:,:,:,j,:));
end
```

Interpolate to find the top/bottom faces `Yface` for every x and interior z.

```
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.

```
  j = max(1,min(1:Ny,Ny-ceil(py/2))-floor(py/2));
  Uface = F(:,:,:,:,:,:,j,:,py+1);
  for q = py:-1:1
    Uface = F(:,:,:,:,:,:,j,:,q) ...
    +(Yface-Y(:,:,:,:,:,:,j+q-1,:)).*Uface;
  end
```

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

```
u(:,1 ,iz,:,patches.bo,:,:,:) = Uface(:,1,:,:,:,:,:,:);
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.

```
  F = nan(nx,ny,patches.EdgyInt+1,nVars,nEnsem,Nx,Ny,Nz,pz+1);
  if patches.EdgyInt % interpolate next-to-face values
    F(:,:,:,:,:,:,:,:,1) = u(:,:,[nz-1 2],:,:,:,:,:);
    Z = z(:,:,[nz-1 2],:,:,:,:,:);
  else % interpolate mid-patch cross-patch values
    F(:,:,:,:,:,:,:,:,1) = u(:,:,k0,:,:,:,:,:);
    Z = z(:,:,k0,:,:,:,:,:);
  end%if patches.EdgyInt
```

Form tables of divided differences.

```
for q = 1:pz
  k = 1:Nz-q;
  F(:,:,:,:,:,:,:,k,q+1) ...
  = ( F(:,:,:,:,:,:,:,k+1,q)-F(:,:,:,:,:,:,:,k,q)) ...
   ./(Z(:,:,:,:,:,:,:,k+q)  -Z(:,:,:,:,:,:,:,k));
end
```

Interpolate to find the face-values on front/back faces `Zface` for every x, y.

```
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.

```
  k = max(1,min(1:Nz,Nz-ceil(pz/2))-floor(pz/2));
  Uface = F(:,:,:,:,:,:,:,k,pz+1);
  for q = pz:-1:1
    Uface = F(:,:,:,:,:,:,:,k,q) ...
    +(Zface-Z(:,:,:,:,:,:,:,k+q-1)).*Uface;
  end
```

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

```
u(:,:,1 ,:,patches.fr,:,:,:) = Uface(:,:,1,:,:,:,:,:);
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`.

```
if isfield(patches,'intTest')&&patches.intTest
else % usual case
    u( 1,:,:,:,:, 1,:,:) = nan;
    u(nx,:,:,:,:,Nx,:,:) = nan;
    u(:, 1,:,:,:,:, 1,:) = nan;
    u(:,ny,:,:,:,:,Ny,:) = nan;
    u(:,:, 1,:,:,:,:, 1) = nan;
    u(:,:,nz,:,:,:,:,Nz) = nan;
end%if
```

End of the non-periodic interpolation code.

```
end%if patches.periodic else
```

Unfold multiple edges No need to restore x, y, z.

```
if mean(patches.nEdge)>1
  nVars = nVars/(mx*my*mz);
  u = reshape( u ,nx,ny,nz,mx,my,mz,nVars,nEnsem,Nx,Ny,Nz);
  nx = nx*mx;
  ny = ny*my;
  nz = nz*mz;
  u = reshape( permute(u,[4 1 5 2 6 3 7:11]) ...
             ,nx,ny,nz,nVars,nEnsem,Nx,Ny,Nz);
end%if patches.nEdge
```

Fin, returning the 8D array of field values with interpolated faces.

```
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.

```
mPeriod = randi([2 3],1,3)
cHetr = exp(0.3*randn([mPeriod 3]));
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.

```
nSubP=mPeriod+2;
nPatch=[5 5 5];
configPatches3(@heteroDiff3, [-pi pi], nan, nPatch ...
    ,0, 0.3, nSubP, 'EdgyInt',true  ...
    ,'hetCoeffs',cHetr );
```

5.4.1 Simulate heterogeneous diffusion

Set initial conditions of a simulation as shown in Figure 5.3.

```
global patches
u0 = exp(-patches.x.^2/4-patches.y.^2/2-patches.z.^2);
u0 = u0.*(1+0.3*rand(size(u0)));
```

Integrate using standard integrators, unevenly spaced in time to better display transients.

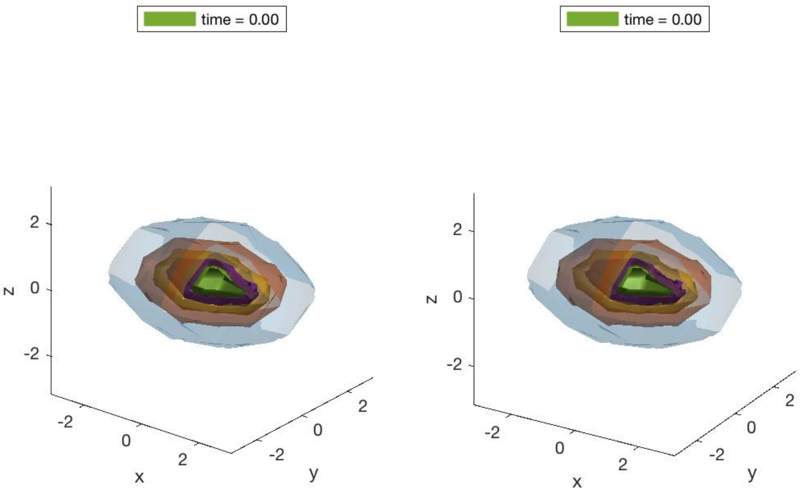
```
if ~exist('OCTAVE_VERSION','builtin')
    [ts,us] = ode23(@patchSys3, 0.3*linspace(0,1,50).^2, u0(:));
else % octave version
    [ts,us] = odeOcts(@patchSys3, 0.3*linspace(0,1).^2, u0(:));
end
```

Plot the solution as an animation over time.

```
figure(1), clf
rgb=get(gca,'defaultAxesColorOrder');
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 $u = 0.1, 0.3, \ldots, 0.9$, with the front quadrant omitted so you can see inside. Figure 5.4 plots the isosurfaces of the computed field at time $t = 0.3$.*




```
x = reshape( patches.x([2:end-1],:,:,:) ,[],1);
y = reshape( patches.y(:,[2:end-1],:,:) ,[],1);
z = reshape( patches.z(:,:,[2:end-1],:) ,[],1);
```

For every time step draw the surface and pause for a short display.

```
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.

```
  u = reshape( us(i,:) ,[nSubP nPatch]);
  u = u([2:end-1],[2:end-1],[2:end-1],:,:,:);
  u = reshape( permute(u,[1 4 2 5 3 6]) ...
      , [numel(x) numel(y) numel(z)]);
```

Optionally cut-out the front corner so we can see inside.

```
  u( (x>0) & (y'<0) & (shiftdim(z,-2)>0) ) = nan;
```

The `isosurface` function requires us to transpose x and y.

```
v = permute(u,[2 1 3]);
```

Draw cross-eyed stereo view of some isosurfaces.

```
  clf;
  for p=1:2
    subplot(1,2,p)
    for iso=5:-1:1
       isov=(iso-0.5)/5;
       hsurf(iso) = patch(isosurface(x,y,z,v,isov));
       isonormals(x,y,z,v,hsurf(iso))
       set(hsurf(iso) ,'FaceColor',rgb(iso,:) ...
           ,'EdgeColor','none' ...
           ,'FaceAlpha',iso/5);
       hold on
    end
    axis equal, view(45-7*p,25)
    axis(pi*[-1 1 -1 1 -1 1])
    xlabel('$x$'), ylabel('$y$'), zlabel('$z$')
    legend(['time = ' num2str(ts(i),'%4.2f')],'Location','north')
    camlight, lighting gouraud
    hold off
  end% each p
  if i==1 % pause for the viewer
       makeJpeg=false;
       if makeJpeg, print(['Figs/' mfilename 't0'],'-djpeg'), end
       disp('Press any key to start animation of isosurfaces')
       pause
  else pause(0.05)
  end
```

Finish the animation loop, and optionally output the isosurfaces of the final field, Figure 5.4.

```
end%for over time
if makeJpeg, print(['Figs/' mfilename 'tFin'],'-djpeg'), end
```

5.4.2 Compute Jacobian and its spectrum

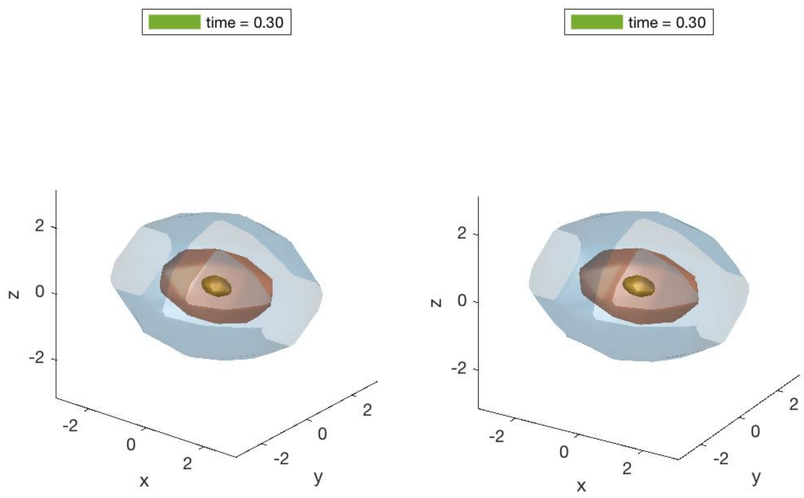
Let's explore the Jacobian dynamics for a range of orders of interpolation, all for the same random patch design and heterogeneity. Except here use a small ratio as we do not plot and then the scale separation is clearest.

```
ratio = 0.025*(1+rand(1,3))
nSubP=randi([3 5],1,3)
nPatch=[3 3 3]
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.

```
    u0 = zeros([nSubP,1,nEnsem,nPatch]);
    u0([1 end],:,:,:) = nan;
    u0(:,[1 end],:,:) = nan;
    u0(:,:,[1 end],:) = 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 $u = 0.1, 0.3, \ldots, 0.9$, with the front quadrant omitted so you can see inside.*




```
    i = find(~isnan(u0));
    sizeJacobian = length(i)
    assert(sizeJacobian<4000 ...
        ,'Jacobian is too big to quickly generate and analyse')
```

Store this many eigenvalues in array across different orders of interpolation.

```
nLeadEvals=prod(nPatch)+max(nPatch);
leadingEvals=[];
```

Evaluate eigenvalues for spectral as the base case for polynomial interpolation of order $2, 4, \ldots$.

```
maxords=6;
for ord=0:2:maxords
    ord=ord
```

Configure with same heterogeneity.

```
    configPatches3(@heteroDiff3,[-pi pi],nan,nPatch ...
        ,ord,ratio,nSubP,'EdgyInt',true,'nEnsem',nEnsem ...
        ,'hetCoeffs',cHetr);
```

Construct the Jacobian of the scheme as the matrix of the linear transformation, obtained by transforming the standard unit vectors.

```
    jac = nan(length(i));
    for j = 1:length(i)
```

```
      u = u0(:)+(i(j)==(1:numel(u0))');
      tmp = patchSys3(0,u);
      jac(:,j) = tmp(i);
    end
```

Test for symmetry, with error if we know it should be symmetric.

```
    notSymmetric=norm(jac-jac')
%    if notSymmetric>1e-7, spy(abs(jac-jac')>1e-7), end%??
    assert(notSymmetric<1e-7,'failed symmetry')
```

Find all the eigenvalues (as `eigs` is unreliable), and put eigenvalues in a vector.

```
    [evecs,evals] = eig((jac+jac')/2,'vector');
    biggestImag=max(abs(imag(evals)));
    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.

```
    [~,k] = sort(-real(evals));
    evals=evals(k); evecs=evecs(:,k);
    if ord==0, nZeroEv=sum(abs(evals(:))<1e-5), end
%    if ord==0, evec0=evecs(:,1:nZeroEv*nLeadEvals);
%    else % find evec closest to that of each leading spectral
%        [~,k]=max(abs(evecs'*evec0));
%        evals=evals(k); % re-sort in corresponding order
%    end
    leadingEvals=[leadingEvals evals(nZeroEv*(1:nLeadEvals))];
end
disp('     spectral    quadratic      quartic  sixth-order ...')
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^x_{ijk}, c^y_{ijk} and c^z_{ijk}, 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.

```
function ut = heteroDiff3(t,u,patches)
  if nargin<3, global patches, end
```

Microscale space-steps. Q: is using `i,j,k` slower than `2:end-1`??

```
  dx = diff(patches.x(2:3));  % x micro-scale step
  dy = diff(patches.y(2:3));  % y micro-scale step
```

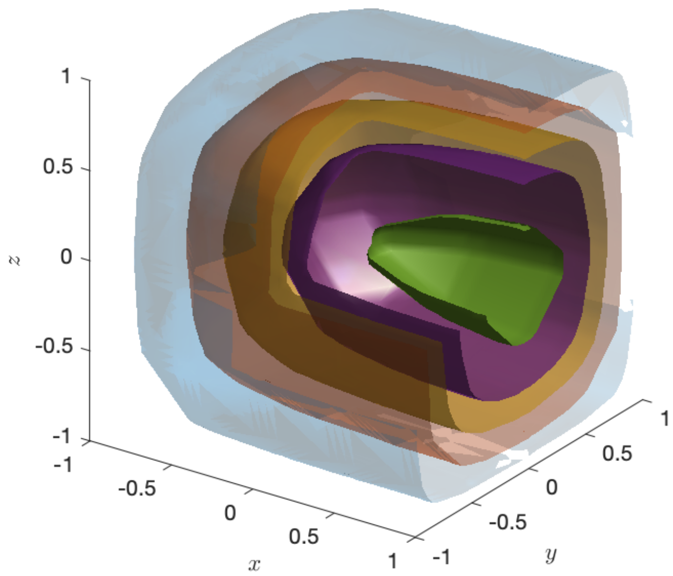
```
  dz = diff(patches.z(2:3));  % z micro-scale step
  i = 2:size(u,1)-1; % x interior points in a patch
  j = 2:size(u,2)-1; % y interior points in a patch
  k = 2:size(u,3)-1; % y interior points in a patch
```

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)`

```
  ut = nan+u; % reserve storage
  ut(i,j,k,:,:,:,:,:) ...
  = diff(patches.cs(:,j,k,1,:).*diff(u(:,j,k,:,:,:,:,:),1),1)/dx^2 ...
   +diff(patches.cs(i,:,k,2,:).*diff(u(i,:,k,:,:,:,:,:),1,2),1,2)/dy^2 ...
   +diff(patches.cs(i,j,:,3,:).*diff(u(i,j,:,:,:,:,:,:),1,3),1,3)/dz^2;
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.

```
clear all
global patches
%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.

```
mPeriod = randi([2 3],1,3)
cDiff = exp(0.3*randn([mPeriod 3]));
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.

```
nSubP = mPeriod+2;
nPatch = 5;
Dom.type = 'equispace';
Dom.bcOffset = zeros(2,3);  Dom.bcOffset(2) = 0.5;
configPatches3(@microDiffBdry3, [-1 1], Dom ...
    , nPatch, 0, 0.05, nSubP, 'EdgyInt',true  ...
    ,'hetCoeffs',cDiff );
```

Set forcing, and store in global patches for access by the microcode

```
patches.fu = 10*exp(-patches.x.^2-patches.y.^2-patches.z.^2);
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.

```
u0 = zeros([nSubP,1,1,nPatch,nPatch,nPatch]);
u0([1 end],:,:,:) = nan;
u0(:,[1 end],:,:) = nan;
u0(:,:,[1 end],:) = nan;
patches.i = find(~isnan(u0));
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).

```
disp('Solving system, takes 10--40 secs'),tic
uSoln = fsolve(@theRes,u0(patches.i) ...
        ,optimoptions('fsolve','Display','off'));
solveTime = toc
normResidual = norm(theRes(uSoln))
normSoln = norm(uSoln)
```

Store the solution into the patches, and give magnitudes.

```
u0(patches.i) = uSoln;
u0 = patchEdgeInt3(u0);
```

Plot isosurfaces of the solution

```
figure(1), clf
rgb=get(gca,'defaultAxesColorOrder');
```

Reshape spatial coordinates of patches.

```
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.

```
u = reshape( permute(squeeze(u0),[2 5 1 4 3 6]) ...
           , [numel(y) numel(x) numel(z)]);
maxu=max(u(:)),  minu=min(u(:))
```

Optionally cut-out the front corner so we can see inside.

```
  u( (x'>0) & (y<0) & (shiftdim(z,-2)>0) ) = nan;
```

Draw some isosurfaces.

```
clf;
for iso=5:-1:1
   isov=(iso-0.5)/5*(maxu-minu)+minu;
   hsurf(iso) = patch(isosurface(x,y,z,u,isov));
   isonormals(x,y,z,u,hsurf(iso))
   set(hsurf(iso) ,'FaceColor',rgb(iso,:) ...
       ,'EdgeColor','none' ,'FaceAlpha',iso/5);
   hold on
end
hold off
axis equal, axis([-1 1 -1 1 -1 1]), view(35,25)
xlabel('$x$'), ylabel('$y$'), zlabel('$z$')
camlight, lighting gouraud
ifOurCf2eps(mfilename) %optionally save plot
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^x_{ijk}, c^y_{ijk} and c^z_{ijk}, 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.

```
function ut = microDiffBdry3(t,u,patches)
  if nargin<3, global patches, end
```

Microscale space-steps.

```
  dx = diff(patches.x(2:3));  % x micro-scale step
  dy = diff(patches.y(2:3));  % y micro-scale step
  dz = diff(patches.z(2:3));  % z micro-scale step
  i = 2:size(u,1)-1; % x interior points in a patch
  j = 2:size(u,2)-1; % y interior points in a patch
  k = 2:size(u,3)-1; % y 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).

```
  u( 1 ,:,:,:,:, 1 ,:,:)=0; %left face of leftmost patch
  u(end,:,:,:,:,end,:,:)=u(end-1,:,:,:,:,end,:,:); %right face of rightmost
```

```
  u(:, 1 ,:,:,:,:, 1 ,:)=0; %bottom face of bottommost
  u(:,end,:,:,:,:,end,:)=0; %top face of topmost
  u(:,:, 1 ,:,:,:,:, 1 )=0; %front face of frontmost
  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)`

```
  ut = nan+u; % reserve storage
  ut(i,j,k,:) ...
  = diff(patches.cs(:,j,k,1).*diff(u(:,j,k,:),1,1),1,1)/dx^2 ...
   +diff(patches.cs(i,:,k,2).*diff(u(i,:,k,:),1,2),1,2)/dy^2 ...
   +diff(patches.cs(i,j,:,3).*diff(u(i,j,:,:),1,3),1,3)/dz^2 ...
   +patches.fu(i,j,k);
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

$$u_{tt} = -\nabla^2(C\nabla^2 u)$$

for microscale variations in scalar $C(x, y, z)$.

Initialise some Matlab aspects.

```
clear all
cMap=jet(64); cMap=0.8*cMap(7:end-7,:); % set colormap
basename = [num2str(floor(1e5*rem(now,1))) mfilename]
%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.

```
mPeriod = [2 2 2];
cHetr = exp(0.9*randn(mPeriod));
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.)

```
global patches
patches = configPatches3(@heteroDispWave3,[-pi pi] ...
    ,'periodic', 5, 0, 0.22, mPeriod+4 ,'EdgyInt',true ...
    ,'hetCoeffs',cHetr ,'nEdge',2);
```

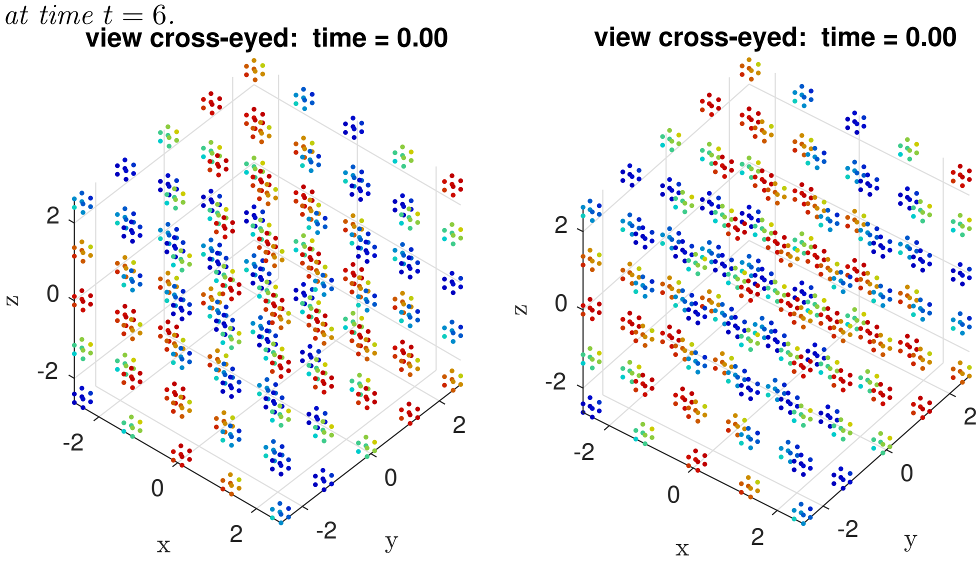
Set a wave initial state using auto-replication of the spatial grid, and as Figure 5.6 shows. This wave propagates diagonally across space. Concatenate the two u, v-fields to be the two components of the fourth dimension.

```
u0 = 0.5+0.5*sin(patches.x+patches.y+patches.z);
v0 =    -0.5*cos(patches.x+patches.y+patches.z)*3;
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).

```
disp('Simulate heterogeneous wave u_tt=delsq[C*delsq(u)]')
tic
[ts,us] = ode23(@patchSys3,linspace(0,6),uv0(:));
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.

```
%%
figure(1), clf, colormap(cMap)
xs = patches.x+0*patches.y+0*patches.z;
ys = patches.y+0*patches.x+0*patches.z;
zs = patches.z+0*patches.y+0*patches.x;
if 1, xs([1:2 end-1:end],:,:,:)=nan;
      xs(:,[1:2 end-1:end],:,:)=nan;
      xs(:,:,[1:2 end-1:end],:)=nan;
end;%option
j=find(~isnan(xs));
```

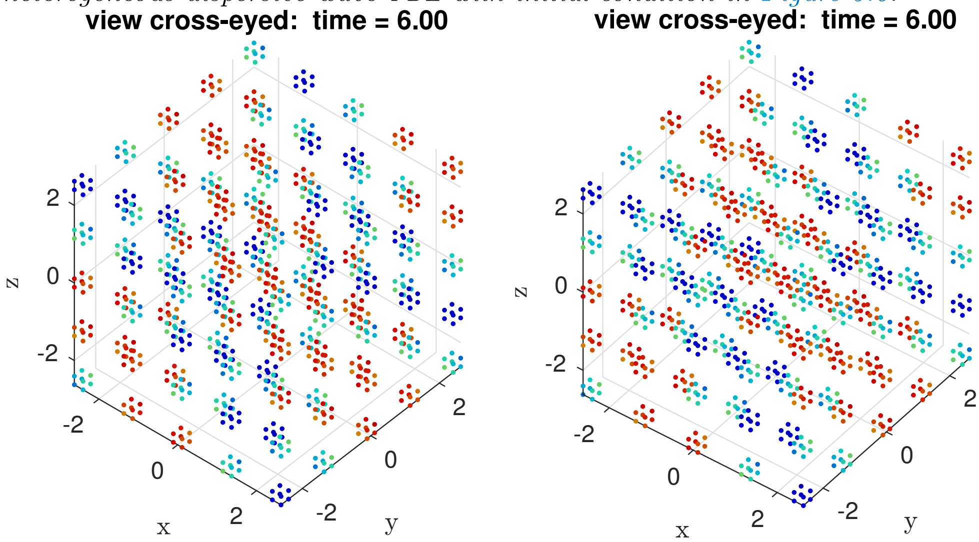
In the scatter plot, `col()` maps the u-data values to the colour of the dots.

```
col = @(u) sign(u).*abs(u);
```

Loop to plot at each and every time step.

```
for i = 1:length(ts)
  uv = patchEdgeInt3(us(i,:));
  u = uv(:,:,:,1,:);
  for p=1:2
    subplot(1,2,p)
    if (i==1)
      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.*




```
      axis equal, caxis(col([0 1])), view(45-4*p,42)
      xlabel('$x$'), ylabel('$y$'), zlabel('$z$')
    end
    title(['view cross-eyed:  time = ' num2str(ts(i),'%4.2f')])
    set( scat(p),'CData',col(u(j)) );
  end
```

Optionally save the initial condition to graphic file for Figure 5.6, and optionally save the last plot.

```
  if i==1,
    ifOurCf2eps([basename 'ic'])
    disp('Type space character to animate simulation')
    pause
  else pause(0.1)
  end
end% i-loop over all times
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 `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 3D array of heterogeneous coefficients, C_{ijk}, c^y_{ijk} and c^z_{ijk}, have been stored in `patches.cs` (3D).

Supply patch information as a third argument (required by parallel computation), or otherwise by a global variable.

```
function ut = heteroDispWave3(t,u,patches)
  if nargin<3, global patches, end
```

Micro-grid space steps.

```
dx = diff(patches.x(2:3));
dy = diff(patches.y(2:3));
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.

```
I = 2:size(u,1)-1; J = 2:size(u,2)-1;  K = 2:size(u,3)-1;
u(I,J,K,1,:) = patches.cs(I,J,K,1,:).*( diff(u(:,J,K,1,:),2,1)/dx^2 ...
    +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.

```
ut = nan+u;  % preallocate output array
i = I(2:end-1); j = J(2:end-1);  k = K(2:end-1);
ut(i,j,k,1,:) = u(i,j,k,2,:);  % du/dt=v
% dv/dt=delta^2 of above C*delta^2
ut(i,j,k,2,:) = -( diff(u(I,j,k,1,:),2,1)/dx^2 ...
  +diff(u(i,J,k,1,:),2,2)/dy^2 +diff(u(i,j,K,1,:),2,3)/dz^2 );
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.

```
clear all, close all
global patches
nRealise = 10
```

5.6.2.1 Check divided difference interpolation

```
fprintf('\n\n**** Check divided difference interpolation\n')
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.)

```
maxErrors=[];
for realisation = 1:nRealise
    nEdge = randi(3,1,3)% =1,2, or 3
    edgyInt = (rand>0.5)
    Lx = 1+3*rand; Ly = 1+3*rand; Lz = 1+3*rand;
    xyzLim = [0 Lx 0 Ly 0 Lz]-[rand*[1 1] rand*[1 1] rand*[1 1]]
    nSubP = nEdge.*( (2-edgyInt)*randi(2,1,3)+1+edgyInt )
    ordCC = 2*randi(3)
    nPatch = ordCC+randi(4,1,3)
    dx = [Lx Ly Lz]./nPatch./nSubP.*rand(1,3)/2
    configPatches3(@sin,xyzLim,'equispace',nPatch,ordCC ...
        ,dx,nSubP,'EdgyInt',edgyInt,'nEdge',nEdge);
```

Second, displace patches to a random non-uniform spacing.

```
Hx = diff(patches.x(1,1,1,:,:,1:2,1,1));
patches.x = patches.x+0.8*Hx*(rand(1,1,1,1,1,nPatch(1),1,1)-0.5);
Hx = squeeze( diff(patches.x(1,1,1,:,:,:,1,1)) )';% for information only
Hy = diff(patches.y(1,1,1,:,:,1,1:2,1));
patches.y = patches.y+0.8*Hy*(rand(1,1,1,1,1,1,nPatch(2),1)-0.5);
Hy = squeeze( diff(patches.y(1,1,1,:,:,1,:,1)) )';% for information only
Hz = diff(patches.z(1,1,1,:,:,1,1,1:2));
patches.z = patches.z+0.8*Hz*(rand(1,1,1,1,1,1,1,nPatch(3))-0.5);
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.

```
    ox=min(ordCC,nPatch(1)-1);
    oy=min(ordCC,nPatch(2)-1);
    oz=min(ordCC,nPatch(3)-1);
    [ps,qs,rs]=ndgrid(0:ox,0:oy,0:oz);
    ps=reshape(ps,1,1,1,[]);
    qs=reshape(qs,1,1,1,[]);
    rs=reshape(rs,1,1,1,[]);
    cs=2*rand(size(ps))-1;
    u0=cs.*patches.x.^ps.*patches.y.^qs.*patches.z.^rs;
```

Then evaluate the interpolation, setting faces to `inf` for error checking.

```
    u=u0;
    u([1:nEdge(1)  end-nEdge(1)+1:end],:,:,:)=inf;
    u(:,[1:nEdge(2)  end-nEdge(2)+1:end],:,:)=inf;
    u(:,:,[1:nEdge(3)  end-nEdge(3)+1:end],:)=inf;
    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.

```
    error = ui-u0;
    hist(log10(abs(error(abs(error)>1e-20))),-20:-6)
    xlabel('log10 error'), pause(0.3)%??
    maxError=max(abs(error(:)))
    maxErrors=[maxErrors maxError];
    assert(maxError<1e-10*4^ordCC ...
    ,'failed divided difference interpolation')
    disp('*** This divided difference test passed')
```

End the for-loops over various parameters.

```
end% for realisation
maxMaxErrorDividedDiffs = max(maxErrors)
disp('***** Passed all divided difference interpolation')
pause(1)
```

5.6.2.2 Test standard spectral interpolation

```
fprintf('\n\n**** Test standard spectral interpolation\n')
pause(1)
```

Test over various numbers of patches, random domain lengths and random ratios. Try realisations of random tests.

```
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.

```
nEdge=randi(3,1,3)% =1,2, or 3
edgyInt = (rand>0.5)
Lx = 1+3*rand, Ly = 1+3*rand, Lz = 1+3*rand
xyzLim = [0 Lx 0 Ly 0 Lz]-[rand*[1 1] rand*[1 1] rand*[1 1]]
nSubP = nEdge.*( (2-edgyInt)*randi(3,1,3)+1+edgyInt )
nPatch = randi([3 6],1,3)
dx = [Lx Ly Lz]./nPatch./nSubP.*rand(1,3)/2
configPatches3(@sin,xyzLim,'periodic',nPatch,0 ...
    ,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.

```
nV=randi(3)
[nx,Nx]=size(squeeze(patches.x));
[ny,Ny]=size(squeeze(patches.y));
[nz,Nz]=size(squeeze(patches.z));
u0=nan(nx,ny,nz,nV,1,Nx,Ny,Nz);
for iV=1:nV
```

```
  ks=floor( rand(1,3).*floor(([Nx Ny Nz]+1)/2) )
  phis = pi*rand(1,3).*(2*ks~=[Nx Ny Nz])
  % generate 8D array via auto-replication
  u0(:,:,:,iV,1,:,:,:)=sin(2*pi*ks(1)*patches.x/Lx+phis(1)) ...
                     .*sin(2*pi*ks(2)*patches.y/Ly+phis(2)) ...
                     .*sin(2*pi*ks(3)*patches.z/Lz+phis(3));
end
```

Copy and `nan` the faces, then interpolate

```
u=u0;
u([1:nEdge(1)  end-nEdge(1)+1:end],:,:,:)=nan;
u(:,[1:nEdge(2)  end-nEdge(2)+1:end],:,:)=nan;
u(:,:,[1:nEdge(3)  end-nEdge(3)+1:end],:)=nan;
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.

```
error = u-u0;
assert(all(~isnan(error(:))),'found nans in the error!')
hist(log10(abs(error(abs(error)>1e-20))),-20:-6)
xlabel('log10 error'), pause(0.3)%??
normError=norm(error(:))
assert(normError<1e-10, '3D spectral interpolation failed')
disp('*** This spectral test passed')
```

End the for-loop over realisations

```
end
disp('***** All the spectral tests passed')
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.)

```
for realisations=1:nRealise
    nEdge = randi(3,1,3)% =1,2, or 3
    edgyInt = (rand>0.5)
    nSubP = nEdge.*( (2-edgyInt)*randi(2,1,3)+1+edgyInt )
    ordCC = 2*randi(3)
    nPatch = ordCC+randi(3,1,3)
    xyzLim=5*[-rand(1,3); rand(1,3)]
    dx = diff(xyzLim)./nPatch./nSubP.*rand(1,3)/2
    configPatches3(@sin,xyzLim,'periodic',nPatch,ordCC ...
        ,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.

```
    [ps,qs,rs]=meshgrid(0:ordCC);
    ps=reshape(ps,1,1,1,[]);
    qs=reshape(qs,1,1,1,[]);
    rs=reshape(rs,1,1,1,[]);
    cs=2*rand(size(ps))-1;
    u0=cs.*patches.x.^ps.*patches.y.^qs.*patches.z.^rs;
```

Then evaluate the interpolation.

```
    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.

```
    I=ordCC/2+1:nPatch(1)-ordCC/2;
    J=ordCC/2+1:nPatch(2)-ordCC/2;
    K=ordCC/2+1:nPatch(3)-ordCC/2;
    error=ui(:,:,:,:,:,I,J,K)-u0(:,:,:,:,:,I,J,K);
    assert(all(~isnan(error(:))),'found nans in the error!')
    hist(log10(abs(error(abs(error)>1e-20))),-20:-6)
    xlabel('log10 error'), pause(0.3)%??
    normError=norm(error(:))
    assert(normError<5e-8 ...
    ,'failed finite stencil polynomial interpolation')
    disp('*** This finite stencil test passed')
```

End the for-loops over various parameters.

```
end%for realisation
disp('***** Passed all polynomial interpolation tests')
```

5.6.2.4 Finished

If no error messages, then all OK.

```
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

Chapter contents

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 that 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 to 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

Section contents

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

$$\frac{\partial c}{\partial t} = -\mathrm{Pe}\, u(y)\frac{\partial c}{\partial x} + \frac{\partial}{\partial x}\left[\kappa_x(y)\frac{\partial c}{\partial x}\right] + \frac{\partial}{\partial y}\left[\kappa_y(y)\frac{\partial c}{\partial y}\right]. \tag{6.1}$$

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

$$\begin{aligned}\frac{\partial c_{ij}}{\partial t} &= -\mathrm{Pe}\, u(y_j)\frac{c_{i+1,j} - c_{i-1,j}}{2\delta x} + \frac{d_{i,j+1/2} - d_{i,j-1/2}}{\delta y} + \frac{D_{i+1/2,j} - D_{i-1/2,j}}{\delta x}, \\ d_{ij} &:= \kappa_y(y_j)\frac{c_{i,j+1/2} - c_{i,j-1/2}}{\delta y}, \quad D_{ij} := \kappa_x(y_j)\frac{c_{i+1/2,j} - c_{i-1/2,j}}{\delta x}. \end{aligned} \tag{6.2}$$

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.

```
clear all
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.

```
ny = 7
y = linspace(-1,1,2*ny+1);
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.

```
mPeriod = 4
cHetr = shiftdim([3/2 1],-1).*(1-y.^2) ...
        .*exp(0.3*randn([mPeriod 2*ny+1 2]));
```

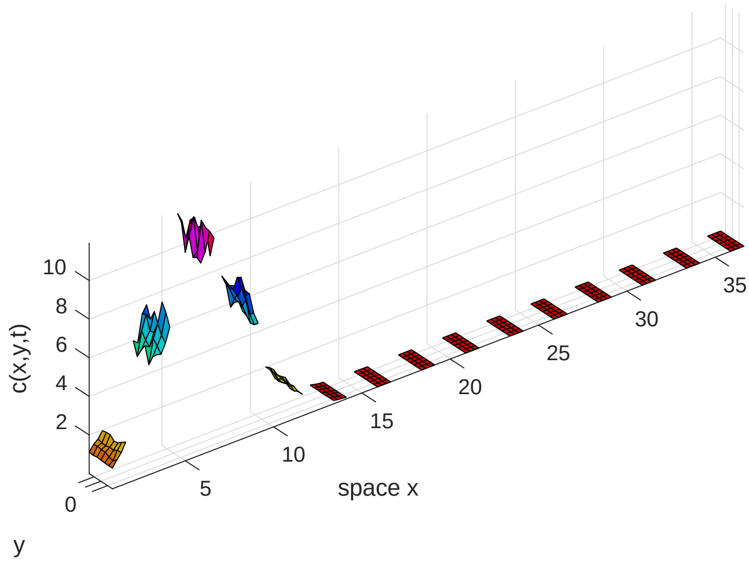
Configure the patch scheme with some arbitrary choices of domain, patches, size ratios. Choose some random order of interpolation to see the alternatives. Set `patches` information to be global so the info can be used for Cases 1–2 without being explicitly passed as arguments. Choose the parallel option if not Case 1, which invokes `spmd`-block internally, so that field variables become *distributed* across cpus.

```
if theCase<=2, global patches, end
nPatch=15
nSubP=2+mPeriod
ratio=0.2+0.2*(theCase<4)
Len=nPatch/ratio
ordCC=2*randi([0 3])
disp('**** Setting configPatches1')
patches = configPatches1(@chanDispMicro, [0 Len], nan ...
    , nPatch, ordCC, ratio, nSubP, 'EdgyInt',true  ...
    ,'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).

```
Peclet = 10
if theCase==1, patches.Pe = Peclet;
else     spmd, patches.Pe = Peclet; end
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.

```
disp('**** Set initial condition and test dc0dt =')
if theCase==1
```

Without parallel processing, invoke the usual operations.

```
    c0 = 10*exp(-(ratio*patches.x-2.5).^2/2) +0*yj;
    c0 = c0.*(1+0.2*rand(size(c0)));
    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`.

```
else, spmd
    c0 = 10*exp(-(ratio*patches.x-2.5).^2/2) +0*yj;
    c0 = c0.*(1+0.2*rand(size(c0),patches.codist));
    dc0dt = patchSys1(0,c0,patches)
    end%spmd
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.

```
warning('Integrating system in time, wait patiently')
ts=4*linspace(0,1);
```

Go to the selected case.

```
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.

```
case 1
%    [cs,uerrs] = RK2mesoPatch(ts,c0);
    [ts,cs] = ode23(@patchSys1,ts,c0(:));
    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.

```
case 2
    cs = RK2mesoPatch(ts,c0);
    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.

```
case 3,spmd
    cs = RK2mesoPatch(ts,c0,[],patches);
    end%spmd
    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.

```
case 4
    microBurst = @(tb0,xb0,bT) ...
        aBurst(tb0 ,reshape(xb0,size(c0)) ,patches);
    ts = 0:0.7:5
    cs = PIRK2(microBurst,ts,gather(c0(:)));
    cs = reshape(cs,[length(ts) size(c0)]);
```

End the four cases.

```
end%switch theCase
```

6.1.2 Plot the solution

Optionally set to save some plots to file.

```
if 0, global OurCf2eps, OurCf2eps=true, end
```

Animate the computed solution field over time

```
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).

```
if theCase==1, x = patches.x;
else, spmd
    x = gather( patches.x );
    end%spmd
    x = x{1};
end
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.

```
nTimes = length(ts)
for l = 1:nTimes
```

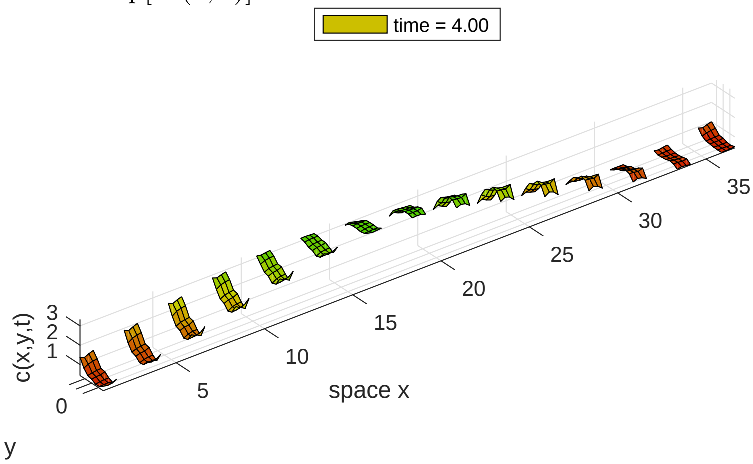
At each time, squeeze sub-patch data into a 3D array, permute to get all the x-variation in the first two dimensions, and reshape into x-variation for each and every (y).

```
  c = reshape( permute( squeeze( ...
      cs(l,:,:,:,:) ) ,[1 3 2]) ,numel(x),ny);
```

Draw surface of each patch, to show both micro-scale and macro-scale variation in space.

```
  if l==1
    hp = surf(x(:),yj,c');
    axis([0 Len -1 1 0 max(c(:))])
    axis equal
    xlabel('space $x$'), ylabel('$y$'); zlabel('$c(x,y,t)$')
    ifOurCf2eps([mfilename 't0'])
    legend(['time = ' num2str(ts(l),'%4.2f')] ...
        ,'Location','north')
    disp('**** pausing, press blank to animate')
    pause
 else
    hp.ZData = c';
    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* $\exp[\mathcal{N}(0, 1)]$.




```
    pause(0.1)
 end
```

Finish the animation loop, and optionally save the final plot to file, Figure 6.2.

```
end%for over time
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.

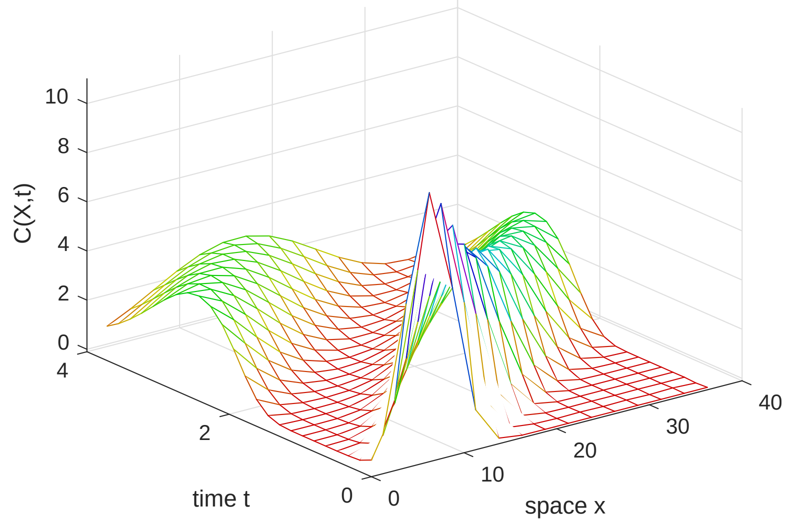
```
figure(2), clf, colormap(0.8*hsv)
X = squeeze(mean(x(2:end-1,:,:,:)));
C = squeeze(mean(mean(cs(:,2:end-1,:,:,:),2),3));
j = 1:ceil(nTimes/30):nTimes;
mesh(X,ts(j),C(j,:));
xlabel('space $x$'),ylabel('time $t$'),zlabel('$C(X,t)$')
zlim([-0.1 11])
ifOurCf2eps([mfilename 'Macro'])
```

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 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.

```
function [tbs,xbs] = aBurst(tb0,xb0,patches)
    normx=max(abs(xb0(:)));
    disp(['* aBurst t=' num2str(tb0) '  |x|=' num2str(normx)])
    assert(normx<20,'solution exploding')
    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.*




```
    spmd
      xb0 = codistributed(xb0,patches.codist);
      xbs = RK2mesoPatch(tbs,xb0,[],patches);
    end%spmd
    xbs=reshape(xbs{1},length(tbs),[]);
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 advections 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).

```
function ct = chanDispMicro(t,c,p)
  [nx,ny,~,~]=size(c); % micro-grid points in patches
  ix = 2:nx-1;         % x interior points in a patch
  dx = diff(p.x(2:3)); % x space step
  dy = 2/ny;           % y space step
  ct = nan+c;          % preallocate output array
  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.

```
  ydif = pcs(ix,1:2:end,2) ...
         .*(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.

```
  ct(ix,:,:,:) = (ydif(:,2:end,:,:)-ydif(:,1:end-1,:,:))/dy ...
  + diff(pcs(:,2:2:end,2).*diff(c))/dx^2 ...
  - p.Pe*pcs(ix,2:2:end,1).*(c(ix+1,:,:,:)-c(ix-1,:,:,:))/(2*dx);
end% function
```

6.2 `rotFilmSpmd`: simulation of a 2D shallow water flow on a rotating heterogeneous substrate

Section contents

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.)

$$\frac{\partial h}{\partial t} = -\nabla \cdot (h\vec{v}), \tag{6.3a}$$

$$\frac{\partial \vec{v}}{\partial t} = \begin{bmatrix} -b & f \\ -f & -b \end{bmatrix} \vec{v} - (\vec{v} \cdot \nabla)\vec{v} - g\nabla h + \vec{\nabla} \cdot (\nu \vec{\nabla} \vec{v}), \tag{6.3b}$$

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.

```
clear all
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.

```
mPeriod = 5
bnu = shiftdim([1 0.5 0.5],-1) ...
      .*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.

```
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.

```
nSubP = 2+mPeriod
nPatch = 9
ratio = 0.2+0.2*(theCase<4)
Len = 2*pi*(1+(theCase==4))
disp('**** Setting configPatches2')
patches = configPatches2(@rotFilmMicro, [0 Len], nan ...
    , nPatch, 4, ratio, nSubP, 'EdgyInt',true  ...
    ,'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.

```
f = 5,  g = 1
if theCase==1, patches.f = f; patches.g = g;
else     spmd, patches.f = f; patches.g = g; end
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.

```
disp('**** Set initial condition and test dhuv0dt =')
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.

```
    huv0 = shiftdim([0.5 0 0],-1) ...
       .*exp(-cos(patches.x)/2-cos(patches.y));
    huv0 = huv0+0.1*shiftdim([0 1 1],-1).*rand(size(huv0));
    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`.

```
else, spmd
    huv0 = shiftdim([0.5 0 0],-1) ...
       .*exp(-cos(patches.x)/2-cos(patches.y));
    huv0 = huv0+0.1*rand(size(huv0),patches.codist);
    dhuv0dt = patchSys2(0,huv0,patches)
    end%spmd
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.

```
warning('Integrating system in time, wait a minute')
ts=0:0.003:0.3;
```

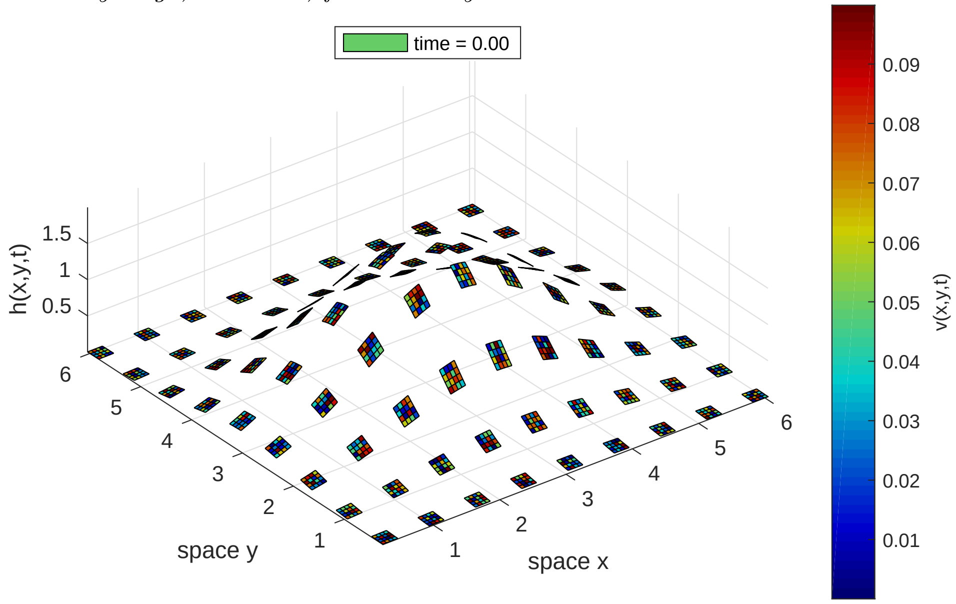
Go to the selected case.

```
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.

   ```
   case 1
   %    tic,[huvs,uerrs] = RK2mesoPatch(ts,huv0);toc
       [ts,huvs] = ode23(@patchSys2,[0 4],huv0(:));
       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.

```
case 2
    huvs = RK2mesoPatch(ts,huv0);
    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.

```
case 3,spmd
    huvs = RK2mesoPatch(ts,huv0,[],patches);
    end%spmd
    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.

```
case 4
    microBurst = @(tb0,xb0,bT) ...
```

```
        aBurst(tb0 ,reshape(xb0,size(huv0)) ,patches);
    ts = 0:0.1:1
    huvs = PIRK2(microBurst,ts,gather(huv0(:)));
    huvs = reshape(huvs,[length(ts) size(huv0)]);
```

End the four cases.

```
end%switch theCase
```

6.2.2 Plot the solution

Optionally set to save some plots to file.

```
if 0, global OurCf2eps, OurCf2eps=true, end
```

Animate the computed solution field over time

```
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).

```
if theCase==1, x = patches.x;
               y = patches.y;
else, spmd
    x = gather( patches.x );
    y = gather( patches.y );
    end%spmd
    x = x{1}; y = y{1};
end
x([1 end],:,:,:,:,:) = nan;
y(:,[1 end],:,:,:,:) = nan;
```

Draw the field values as a patchy surface evolving over 100–200 time steps.

```
nTimes = length(ts)
for l = 1:ceil(nTimes/200):nTimes
```

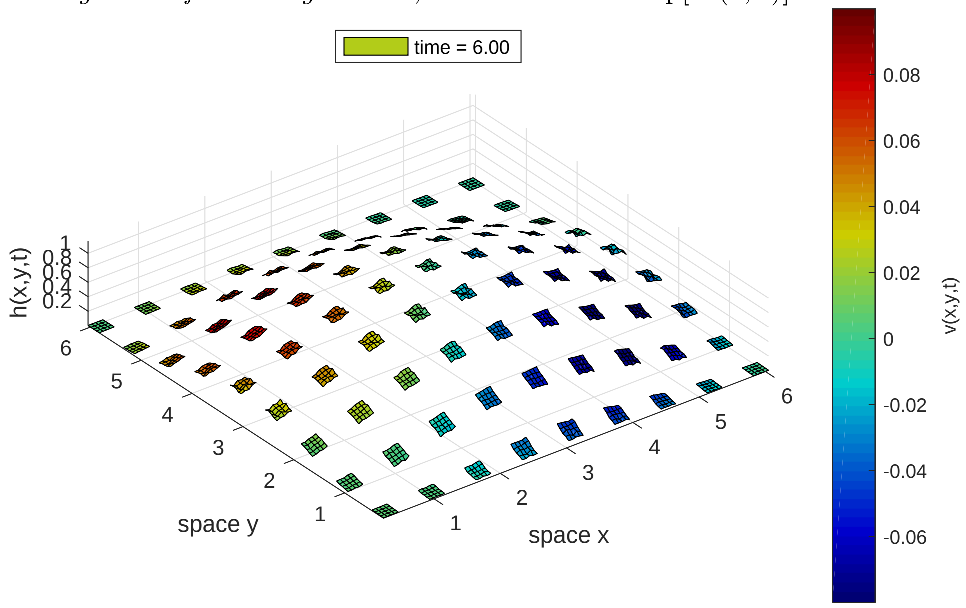
At each time, squeeze sub-patch data fields into three 4D arrays, permute to get all the x/y-variations in the first/last two dimensions, and and then reshape to 2D.

```
  h = reshape( permute( squeeze( ...
      huvs(l,:,:,1,1,:,:) ) ,[1 3 2 4]) ,numel(x),numel(y));
  u = reshape( permute( squeeze( ...
      huvs(l,:,:,2,1,:,:) ) ,[1 3 2 4]) ,numel(x),numel(y));
  v = reshape( permute( squeeze( ...
      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.

```
  if l==1
    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* $\exp[\mathcal{N}(0, 1)]$.




```
    axis([0 Len 0 Len 0 max(h(:))])
    c = colorbar; c.Label.String = 'v(x,y,t)';
    legend(['time = ' num2str(ts(l),'%4.2f')] ...
        ,'Location','north')
    axis equal
    xlabel('space $x$'), ylabel('space $y$'), zlabel('$h(x,y,t)$')
    ifOurCf2eps([mfilename 't0'])
    disp('**** pausing, press blank to begin animation')
    pause
 else
    hp.ZData = h'; hp.CData = v';
    legend(['time = ' num2str(ts(l),'%4.2f')])
    pause(0.1)
 end
```

Finish the animation loop, and optionally save the final plot to file, Figure 6.5.

```
end%for over time
ifOurCf2eps([mfilename 'tFin'])
```

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 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.

```
function [tbs,xbs] = aBurst(tb0,xb0,patches)
    normx=max(abs(xb0(:)));
    disp(['* aBurst t=' num2str(tb0) '  |x|=' num2str(normx)])
    assert(normx<20,'solution exploding')
    tbs = tb0+(0:0.003:0.015);
    spmd
      xb0 = codistributed(xb0,patches.codist);
      xbs = RK2mesoPatch(tbs,xb0,[],patches);
    end%spmd
    xbs=reshape(xbs{1},length(tbs),[]);
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 $\times$ 3): herein `patches` is named `p`.

```
function huvt = rotFilmMicro(t,huv,p)
  [nx,ny,~]=size(huv); % micro-grid points in patches
  i = 2:nx-1;          % x interior points in a patch
  j = 2:ny-1;          % y interior points in a patch
  dx = diff(p.x(2:3)); % x space step
  dy = diff(p.y(2:3)); % y space step
  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.

```
  h=1; u=2; v=3;
  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()`.

```
huv(1,ny,u,:,:,:) = huv(2,ny,u,:,:,:)+huv(1,ny-1,u,:,:,:) ...
                   -huv(2,ny-1,u,:,:,:);
huv(nx,1,v,:,:,:) = huv(nx,2,v,:,:,:)+huv(nx-1,1,v,:,:,:) ...
                   -huv(nx-1,2,v,:,:,:);
v4u = (huv(i,j-1,v,:,:,:)+huv(i+1,j,v,:,:,:) ...
      +huv(i,j,v,:,:,:)+huv(i+1,j-1,v,:,:,:))/4;
```

```
u4v = (huv(i,j+1,u,:,:,:)+huv(i-1,j,u,:,:,:) ...
      +huv(i,j,u,:,:,:)+huv(i-1,j+1,u,:,:,:))/4;
h2u = (huv(2:nx,:,h,:,:,:)+huv(1:nx-1,:,h,:,:,:))/2;
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):

```
  huvt(i,j,h,:,:,:) = ...
    - (h2u(i,j  ,:,:,:,:).*huv(i  ,j,u,:,:,:) ...
      -h2u(i-1,j,:,:,:,:).*huv(i-1,j,u,:,:,:) )/dx ...
    - (h2v(i,j  ,:,:,:,:).*huv(i,j  ,v,:,:,:) ...
      -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):

```
  huvt(i,j,u,:,:,:) = ...
    - p.cs(i,j,b).*huv(i,j,u,:,:,:) + p.f.*v4u ...
    - huv(i,j,u,:,:,:).*(huv(i+1,j,u,:,:,:)-huv(i-1,j,u,:,:,:))/(2*dx) ...
    - v4u.*(huv(i,j+1,u,:,:,:)-huv(i,j-1,u,:,:,:))/(2*dy) ...
    - p.g*(huv(i+1,j,h,:,:,:)-huv(i,j,h,:,:,:))/dx ...
    + diff(p.cs(:,j,nux).*diff(huv(:,j,u,:,:,:),[],1),[],1)/dx^2 ...
    + 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):

```
  huvt(i,j,v,:,:,:) = ...
    - p.cs(i,j,b).*huv(i,j,v,:,:,:) - p.f.*u4v ...
    - u4v.*(huv(i+1,j,v,:,:,:)-huv(i-1,j,v,:,:,:))/(2*dx) ...
    - huv(i,j,v,:,:,:).*(huv(i,j+1,v,:,:,:)-huv(i,j-1,v,:,:,:))/(2*dy) ...
    - p.g*(huv(i,j+1,h,:,:,:)-huv(i,j,h,:,:,:))/dy ...
    + diff(p.cs(:,j,nux).*diff(huv(:,j,v,:,:,:),[],1),[],1)/dx^2 ...
    + diff(p.cs(i,:,nuy).*diff(huv(i,:,v,:,:,:),[],2),[],2)/dy^2 ;
end% function
```

6.3 `homoDiff31spmd`: computational homogenisation of a 1D dispersion via parallel simulation on small 3D patches of heterogeneous diffusion

Section contents

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.

```
clear all
theCase = 1
```

Set micro-scale heterogeneity with various spatial periods in the three directions.

```
mPeriod = [4 3 2] %1+randperm(3)
cHetr = exp(0.3*randn([mPeriod 3]));
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.

```
if any(theCase==[1 2]), global patches, end
nSubP=mPeriod+2
nPatch=[9 1 1]
ratio=0.3
Len=nPatch(1)/ratio
ordCC=2*randi([0 3])
disp('**** Setting configPatches3')
patches = configPatches3(@heteroDiff3,[0 Len 0 1 0 1], nan ...
    , nPatch, ordCC, [ratio 1 1], nSubP, 'EdgyInt',true  ...
    ,'hetCoeffs',cHetr ,'parallel',(theCase>1) );
```

6.3.1 Simulate heterogeneous diffusion

Set initial conditions of a simulation as shown in Figure 6.6.

```
disp('**** Set initial condition and testing du0dt =')
if theCase==1
```

Without parallel processing, invoke the usual operations.

```
    u0 = exp( -(patches.x-Len/2).^2/Len ...
              -patches.y.^2/2-patches.z.^2 );
    u0 = u0.*(1+0.2*rand(size(u0)));
    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`.

```
else, spmd
    u0 = exp( -(patches.x-Len/2).^2/Len ...
              -patches.y.^2/2-patches.z.^2/4 );
    u0 = u0.*(1+0.2*rand(size(u0),patches.codist));
    du0dt = patchSys3(0,u0,patches);
    end%spmd
end%if theCase
```

Integrate in time. Use non-uniform time-steps for fun, and to show more of the initial rapid transients.

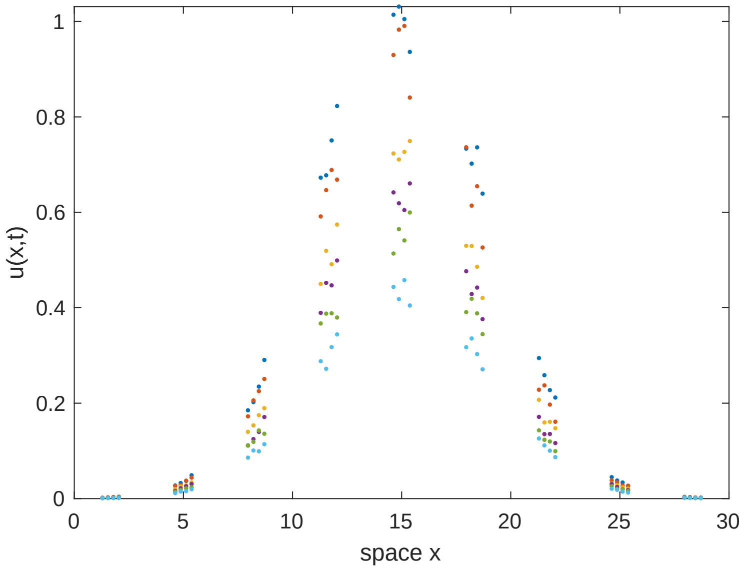
Alternatively, use `RK2mesoPatch` which reduces communication between patches, recalling that, by default, `RK2mesoPatch` does ten micro-steps for each specified step in `ts`. For unit cube patches, need micro-steps less than about 0.004 for stability.

```
warning('Integrating system in time, wait patiently')
ts=0.4*linspace(0,1,21).^2;
```

Go to the selected case.

```
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.

```
case 1
%     [us,uerrs] = RK2mesoPatch(ts,u0);
    [ts,us] = ode23(@patchSys3,ts,u0(:));
    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.

```
case 2
    us = RK2mesoPatch(ts,u0);
    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.

```
case 3,spmd
    us = RK2mesoPatch(ts,u0,[],patches);
    end%spmd
    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.

```
case 4
    microBurst = @(tb0,xb0,bT) ...
        aBurst(tb0 ,reshape(xb0,size(u0)) ,patches);
    ts = 0:3:51
    us = PIRK2(microBurst,ts,gather(u0(:)));
    us = reshape(us,[length(ts) size(u0)]);
```

End the four cases.

```
end%switch theCase
```

6.3.2 Plot the solution

Optionally save some plots to file.

```
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.

```
figure(1), clf
if theCase==1
    x = reshape( patches.x(2:end-1,:,:,:) ,[],1);
else, spmd
    x = reshape(gather( patches.x(2:end-1,:,:,:) ),[],1);
    end%spmd
    x = x{1};
end
```

For every time step draw the field values as dots and pause for a short display.

```
nTimes = length(ts)
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).

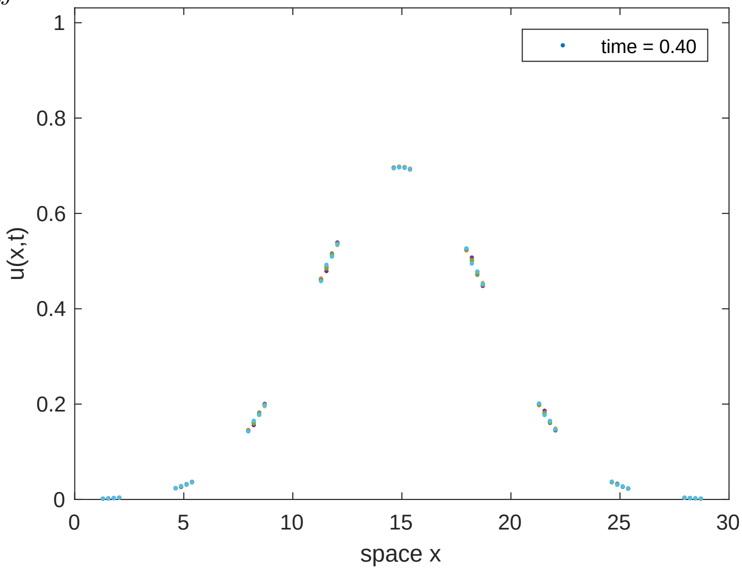
```
  u = reshape( permute( squeeze( ...
      us(l,2:end-1,2:end-1,2:end-1,:) ) ,[1 4 2 3]) ,numel(x),[]);
```

Draw point data to show spread at each cross-section, as well as macro-scale variation in the long space direction.

```
  if l==1
    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.




```
    axis([0 Len 0 max(u(:))])
    xlabel('space $x$'), ylabel('$u(x,y,z,t)$')
    ifOurCf2eps([mfilename 't0'])
    legend(['time = ' num2str(ts(l),'%4.2f')])
    disp('**** pausing, press blank to animate')
    pause
 else
    for p=1:size(u,2), hp(p).YData=u(:,p); end
    legend(['time = ' num2str(ts(l),'%4.2f')])
    pause(0.1)
 end
```

Finish the animation loop, and optionally output the final plot, Figure 6.7.

```
end%for over time
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).

```
function [tbs,xbs] = aBurst(tb0,xb0,patches)
    normx=max(abs(xb0(:)));
    disp(['aBurst t = ' num2str(tb0) '  |x| = ' num2str(normx)])
    assert(normx<10,'solution exploding')
    tbs = tb0+(0:0.02:0.2);
    spmd
      xb0 = codistributed(xb0,patches.codist);
```

```
      xbs = RK2mesoPatch(tbs,xb0,[],patches);
    end%spmd
    xbs=reshape(xbs{1},length(tbs),[]);
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.

```
function [xs,errs] = RK2mesoPatch(ts,x0,nMicro,patches)
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 $\mathbb{R}^\ell$ 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 `configPatches`n and provided as either as parameter, or as a global variable.

Output

- `xs`, 5/7/9D (depending upon `nD`) array of length $\ell \times \cdots$ 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 $\mathbb{R}^\ell$ 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.

```
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??

```
if isequal(class(patches),'Composite') && numlabs==1
    spmd,
      [xs,errs] = RK2mesoPatch(ts,x0,nMicro,patches);
    end% spmd
    assert(isequal(class(xs)  ,'Composite'),' xs  not composite')
    assert(isequal(class(errs),'Composite'),'errs not composite')
    return
end
```

Set the number of space dimensions from the number stored patch-size ratios.

```
nD = length(patches.ratio);
```

Set the micro-time-steps and create storage for outputs.

```
dt = diff(ts)/nMicro;
xs = nan([numel(ts) size(x0)]);
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]

```
switch nD
  case 1, x0 = patchEdgeInt1(x0,patches);
          xs(1,:,:,:,:) = gather(x0);
  case 2, x0 = patchEdgeInt2(x0,patches);
          xs(1,:,:,:,:,:,:) = gather(x0);
  case 3, x0 = patchEdgeInt3(x0,patches);
          xs(1,:,:,:,:,:,:,:,:) = gather(x0);
  end;%switch nD
errs(1) = 0;
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.

```
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.

```
  switch nD
    case 1, dx0 = patchEdgeInt1(f1,patches);
    case 2, dx0 = patchEdgeInt2(f1,patches);
    case 3, dx0 = patchEdgeInt3(f1,patches);
    end;%switch nD
```

Perform the micro-time steps.

```
  for m=1:nMicro
    f0 = f1;
%    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.

```
    switch nD
      case 1, f0([1 end],:,:,:)=dx0([1 end],:,:,:);
      case 2, f0([1 end],:,:,:,:,:)=dx0([1 end],:,:,:,:,:);
              f0(:,[1 end],:,:,:,:)=dx0(:,[1 end],:,:,:,:);
      case 3
        f0([1 end],:,:,:,:,:,:,:)=dx0([1 end],:,:,:,:,:,:,:);
        f0(:,[1 end],:,:,:,:,:,:)=dx0(:,[1 end],:,:,:,:,:,:);
        f0(:,:,[1 end],:,:,:,:,:)=dx0(:,:,[1 end],:,:,:,:,:);
    end;%switch nD
%    assert(iscodistributed(f0),'f0 not codist two')
```

Simple second-order accurate Runge–Kutta micro-scale time-step.

```
    xh = x0+f0*dt(k)/2;
%    assert(iscodistributed(xh),'xh not codist')
    fh = patches.fun(ts(k)+dt(k)*(m-0.5),xh,patches);
%    assert(iscodistributed(fh),'fh not codist one')
    switch nD
      case 1, fh([1 end],:,:,:)=dx0([1 end],:,:,:);
      case 2, fh([1 end],:,:,:,:,:)=dx0([1 end],:,:,:,:,:);
              fh(:,[1 end],:,:,:,:)=dx0(:,[1 end],:,:,:,:);
      case 3
        fh([1 end],:,:,:,:,:,:,:)=dx0([1 end],:,:,:,:,:,:,:);
        fh(:,[1 end],:,:,:,:,:,:)=dx0(:,[1 end],:,:,:,:,:,:);
        fh(:,:,[1 end],:,:,:,:,:)=dx0(:,:,[1 end],:,:,:,:,:);
    end;%switch nD
%    assert(iscodistributed(fh),'fh not codist two')
    x0 = x0+fh*dt(k);
%    assert(iscodistributed(x0),'x0 not codist two')
```

End the burst of micro-time-steps.

```
  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).

```
  switch nD
    case 1, x0 = patchEdgeInt1(x0,patches);
            xs(k+1,:,:,:,:) = gather(x0);
    case 2, x0 = patchEdgeInt2(x0,patches);
            xs(k+1,:,:,:,:,:,:) = gather(x0);
    case 3, x0 = patchEdgeInt3(x0,patches);
            xs(k+1,:,:,:,:,:,:,:,:) = gather(x0);
    end;%switch nD
%  assert(iscodistributed(x0),'x0 not codist three')
  f1 = patches.fun(ts(k+1),x0,patches);
  switch nD
    case 1, f1([1 end],:,:,:)=dx0([1 end],:,:,:);
    case 2, f1([1 end],:,:,:,:,:)=dx0([1 end],:,:,:,:,:);
            f1(:,[1 end],:,:,:,:)=dx0(:,[1 end],:,:,:,:);
    case 3
      f1([1 end],:,:,:,:,:,:,:)=dx0([1 end],:,:,:,:,:,:,:);
      f1(:,[1 end],:,:,:,:,:,:)=dx0(:,[1 end],:,:,:,:,:,:);
      f1(:,:,[1 end],:,:,:,:,:)=dx0(:,:,[1 end],:,:,:,:,:);
    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.

```
  f0=f0-2*fh+f1;
%  assert(iscodistributed(f0),'f2ndDeriv not codist')
  errs(k+1) = sqrt(gather(mean(f0(:).^2,'omitnan')))*dt(k)/6;
end%for-loop
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 camal 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.

```
% input *.m files for ... Author, date
%!TEX root = ../Doc/eqnFreeDevMan.tex
\chapter{...}
\label{ch:...}
\localtableofcontents
Introduction...
\input{../Dir/fun.m} % prefix associated files with 'fun'
\input{../Dir/funExample.m}
...
\begin{devMan}
\section{To do}
...
\section{Miscellaneous tests}
\input{../Dir/funTest.m}
...
\end{devMan}
```

Table A.2: template for a function-section `Dir/*.m` file.

```
% Short explanation for users typing "help fun"
% Author, date
%!TEX root = ../Doc/eqnFreeDevMan.tex
%{
\section{\texttt{...}: ...}
\label{sec:...}
\localtableofcontents
\subsection{Introduction}
Overview LaTeX explanation.
\begin{matlab}
%}
function ...
%{
\end{matlab}
\paragraph{Input} ...
\paragraph{Output} ...
\begin{devMan}
Repeated as desired:
LaTeX between end-matlab and begin-matlab
\begin{matlab}
%}
Matlab code between %} and %{
%{
\end{matlab}
Concluding LaTeX before following final lines.
\end{devMan}
%}
```

Appendix B Aspects of developing a 'toolbox' for patch dynamics

Chapter contents

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 jth 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 $\vec{U}(t) \in \mathbb{R}^{d_{\bar{U}}}$ 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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