

Equation-Free function toolbox for Matlab/Octave: Summary User 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	3
2	Projective integration of deterministic ODEs	5
2.1	Introduction	6
2.2	PIRK2(): projective integration of second-order accuracy	9
2.3	egPIMM: Example projective integration of Michaelis–Menton kinetics	13
2.4	PIG(): Projective Integration via a General macroscale integrator	17
2.5	PIRK4(): projective integration of fourth-order accuracy	21
2.6	cdmc(): constraint defined manifold computing	23
3	Patch scheme for given microscale discrete space system	24
3.1	configPatches1(): configures spatial patches in 1D	28
3.2	patchSys1(): interface 1D space to time integrators	34
3.3	patchEdgeInt1(): sets patch-edge values from interpolation over the 1D macroscale	35
3.4	homogenisationExample: simulate heterogeneous diffusion in 1D	37
3.5	homoDiffEdgy1: computational homogenisation of a 1D heterogeneous diffusion by simulation on small patches	42
3.6	Eckhardt2210eg2: example of a 1D heterogeneous diffusion by simulation on small patches	48
3.7	EckhardtEquilib: find an equilibrium of a 1D heterogeneous diffusion via small patches	52
3.8	EckhardtEquilibErrs: explore errors in equilibria of a 1D heterogeneous diffusion on small patches	54
3.9	Eckhardt2210eg1: example of 1D space-time heterogeneous diffusion via computational homogenisation with projective integration and small patches	59
3.10	homoLanLif1D: computational homogenisation of a 1D heterogeneous Landau–Lifshitz by simulation on small patches	63
3.11	quasiLogAxes(): transforms plot to quasi-log axes	69

3.12	<code>theRes()</code> : wrapper function to zero for equilibria	70
3.13	<code>configPatches2()</code> : configures spatial patches in 2D	71
3.14	<code>patchSys2()</code> : interface 2D space to time integrators	78
3.15	<code>patchEdgeInt2()</code> : sets 2D patch edge values from 2D macroscale interpolation	79
3.16	<code>monoscaleDiffEquil2</code> : equilibrium of a 2D monoscale heterogeneous diffusion via small patches	81
3.17	<code>twoscaleDiffEquil2</code> : equilibrium of a 2D twoscale heterogeneous diffusion via small patches	84
3.18	<code>twoscaleDiffEquil2Errs</code> : errors in equilibria of a 2D twoscale heterogeneous diffusion via small patches	87
3.19	<code>abdulleDiffEquil2</code> : equilibrium of a 2D multiscale heterogeneous diffusion via small patches	94
3.20	<code>randAdvecDiffEquil2</code> : equilibrium of a 2D random heterogeneous advection-diffusion via small patches	97
3.21	<code>homoWaveEdgy2</code> : computational homogenisation of a forced, non-autonomous, 2D wave via simulation on small patches	101
3.22	<code>configPatches3()</code> : configures spatial patches in 3D	106
3.23	<code>patchSys3()</code> : interface 3D space to time integrators	114
3.24	<code>patchEdgeInt3()</code> : sets 3D patch face values from 3D macroscale interpolation	116
3.25	<code>homoDiffEdgy3</code> : computational homogenisation of a 3D diffusion via simulation on small patches	118
3.26	<code>homoDiffBdryEquil3</code> : equilibrium via computational homogenisation of a 3D heterogeneous diffusion on small patches	124
4	Matlab parallel computation of the patch scheme	128
4.1	<code>chanDispSpmd</code> : simulation of a 1D shear dispersion via simulation on small patches across a channel	130
4.2	<code>rotFilmSpmd</code> : simulation of a 2D shallow water flow on a rotating heterogeneous substrate	138
4.3	<code>homoDiff31spmd</code> : computational homogenisation of a 1D dispersion via parallel simulation on small 3D patches of heterogeneous diffusion	146
4.4	<code>RK2mesoPatch()</code>	152

1 Introduction

Users Download via <https://github.com/ua1184615/EquationFreeGit>. Place the folder of this toolbox in a path searched by MATLAB/Octave. Then read the section(s) that documents the function of interest.

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

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

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

- In 1D space adapt the code at the beginning of `configPatches1.m` for Burgers' PDE ([Section 3.1.1](#)).
- In 2D space adapt the code at the beginning of `configPatches2.m` for nonlinear diffusion ([Section 3.13.1](#)).
- In 3D space adapt the code at the beginning of `configPatches3.m` for wave propagation through a heterogeneous medium ([Section 3.22.1](#)), or the patches of the 3D heterogeneous diffusion of `homoDiffEdgy3.m` ([Section 3.25](#)).
- Other provided examples include cases of macroscale *computational homogenisation* of microscale heterogeneity.

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

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

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

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

[Chapter 4](#) provides small examples of how to parallelise the patch computations over multiple processors. But such parallelisation may be only useful for scenarios where the microscale code has many millions of operations per time-step.

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

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

2 Projective integration of deterministic ODEs

Chapter contents

2.1	Introduction	6
2.2	PIRK2(): projective integration of second-order accuracy	9
2.2.1	Introduction	9
2.2.2	If no arguments, then execute an example	11
2.3	egPIMM: Example projective integration of Michaelis–Menton kinetics	13
2.4	PIG(): Projective Integration via a General macroscale integrator	17
2.4.1	Introduction	17
2.4.2	If no arguments, then execute an example	19
2.5	PIRK4(): projective integration of fourth-order accuracy	21
2.5.1	Introduction	21
2.6	cdmc(): constraint defined manifold computing	23

2.1 Introduction

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

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

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

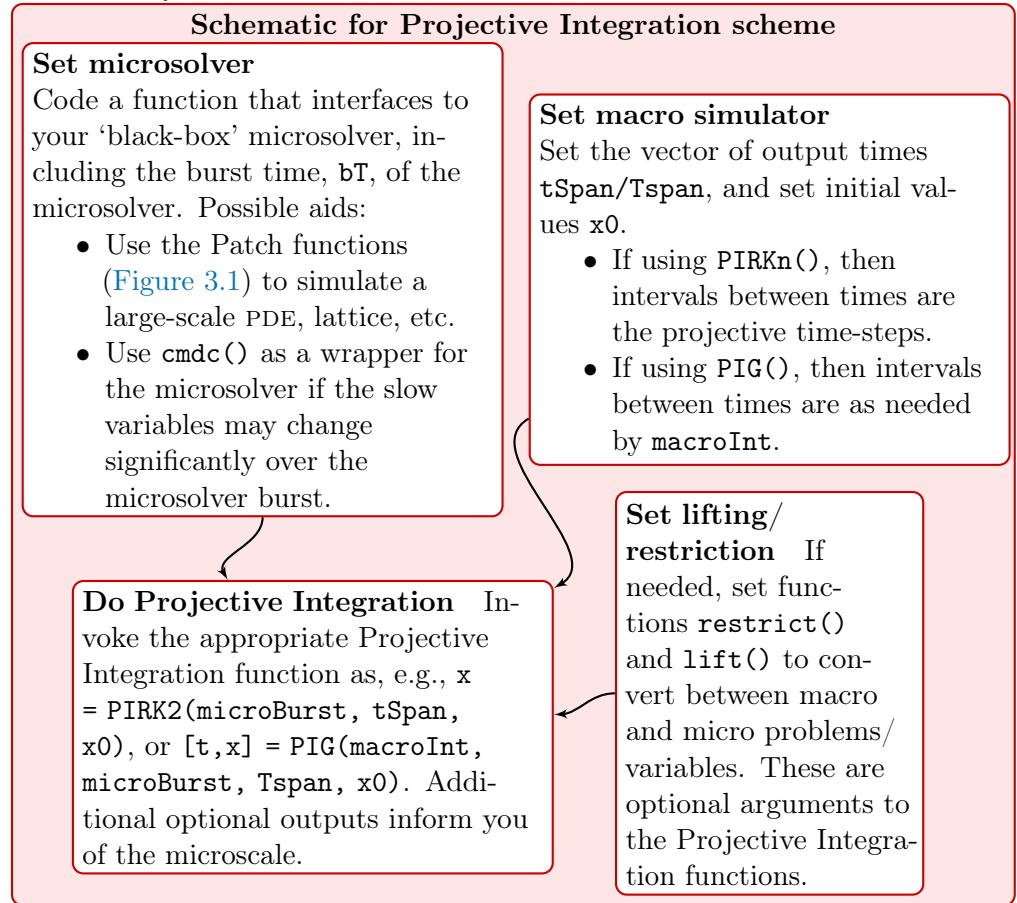
The Projective Integration section of this toolbox consists of several functions. Each function implements over a long-time scale a variant of a standard numerical method to simulate/integrate the emergent dynamics of the complex system. Each function has standardised inputs and outputs.

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

Main functions

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

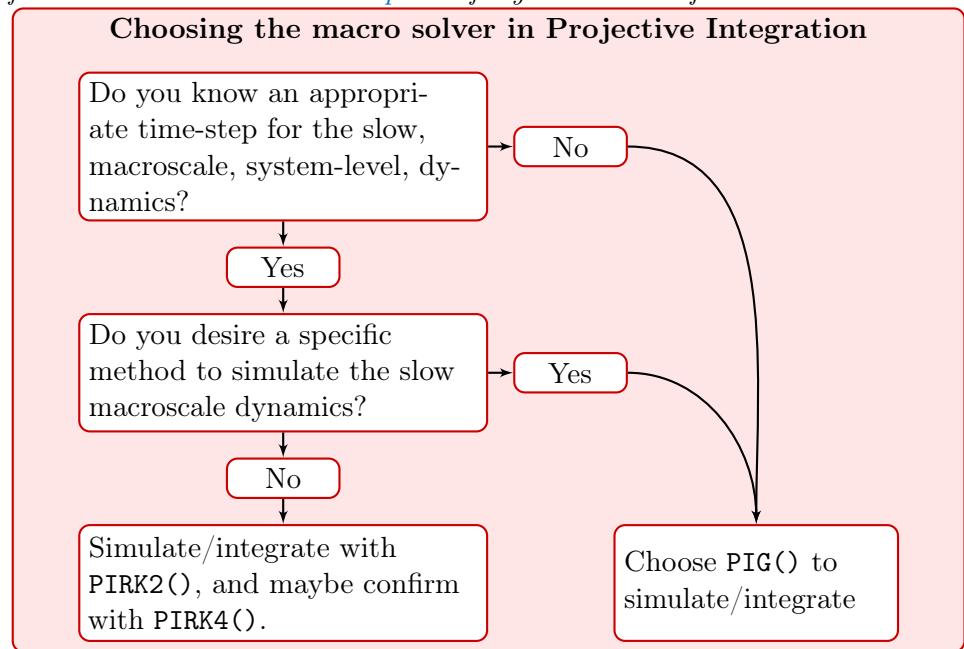
Figure 2.1: The Projective Integration method greatly accelerates simulation/integration of a system exhibiting multiple time scales. The Projective Integration Chapter 2 presents several separate functions, as well as several optional wrapper functions that may be invoked. This chart overviews constructing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



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

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

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



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

Section contents

2.2.1 Introduction	9
2.2.2 If no arguments, then execute an example	11

2.2.1 Introduction

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

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

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

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

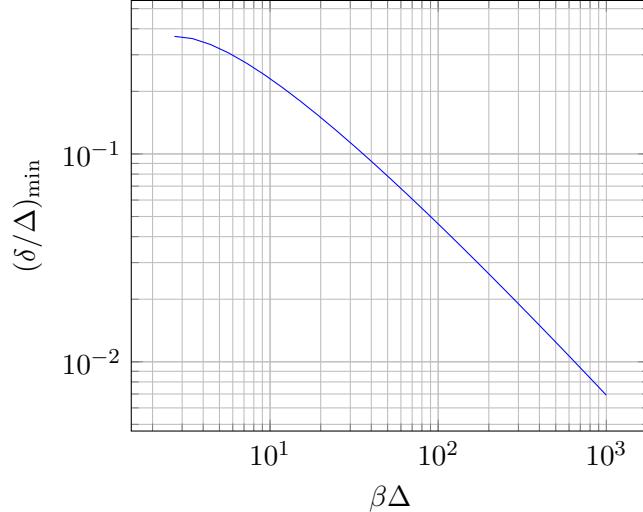
```
[tOut, xOut] = microBurst(tStart, xStart, bT)
```

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

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

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

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 .



slow manifold; else if missing or [], then `microBurst()` must itself determine the length of a burst.

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

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

1. a macroscale time-step, $\Delta = \text{diff}(\text{tSpan})$, such that $\alpha\Delta \approx \sqrt{6\varepsilon}$, and
2. a microscale burst length, $\delta = \text{bT} \gtrsim \frac{1}{\beta} \log |\beta\Delta|$, 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 row is an accurate estimate of the state at the corresponding

time `tms` and helps visualise details of the solution.

- `rm`, optional, a struct containing the ‘remaining’ applications of the microBurst required by the Projective Integration method during the calculation of the macrostep:
 - `rm.t` is a column vector of microscale times; and
 - `rm.x` is the array of corresponding burst states.

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

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

2.2.2 If no arguments, then execute an example

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

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

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

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

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

Upon finishing execution of the example, exit this function.

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

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

```

15 function [ts, xs] = MMburst(ti, xi, bT)
16     global MMepsilon
17     dMMdt = @(t,x) [ -x(1)+(x(1)+0.5)*x(2)
18                      1/MMepsilon*( x(1)-(x(1)+1)*x(2) ) ];
19     if ~exist('OCTAVE_VERSION','builtin')
20         [ts, xs] = ode23(dMMdt, [ti ti+bT], xi);
21     else % octave version
22         [ts, xs] = odeOct(dMMdt, [ti ti+bT], xi);
23     end
24 end

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

```

2.3 egPIMM: Example projective integration of Michaelis–Menton kinetics

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

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

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

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

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

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

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

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

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

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

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

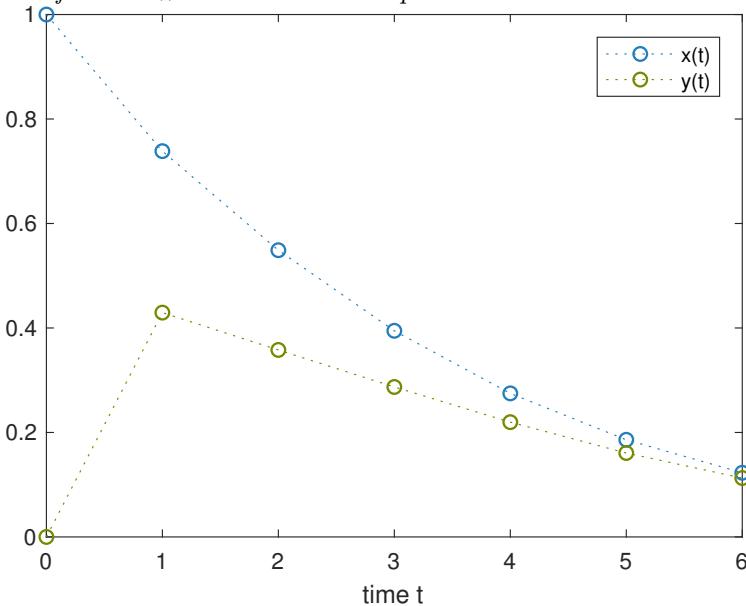


Figure 2.5 plots the macroscale and microscale results—also showing that the initial burst is by default twice as long. Observe the slow variable $x(t)$ is also affected by the initial transient (hence other schemes which ‘freeze’ slow variables are less accurate).

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

```

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

```

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

```

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

```

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

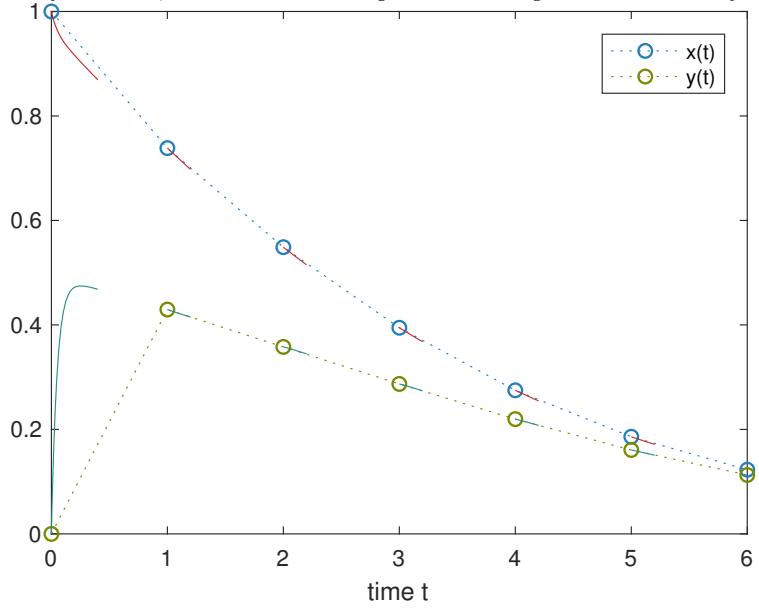
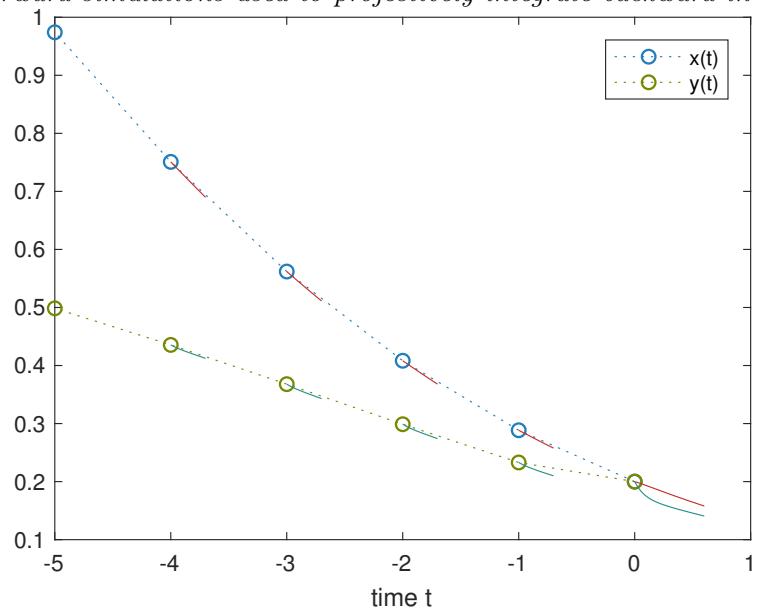


Figure 2.6: Michaelis–Menten enzyme kinetics at $\epsilon = 0.1$ simulated backward with the projective integration of PIRK2(): the microscale bursts show the short forward simulations used to projectively integrate backward in time.



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

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

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

Section contents

2.4.1	Introduction	17
2.4.2	If no arguments, then execute an example	19

2.4.1 Introduction

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

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

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

Inputs:

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

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

where

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

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

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

$$[tbs, xbs] = \text{microBurst}(tb0, xb0)$$

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`'.

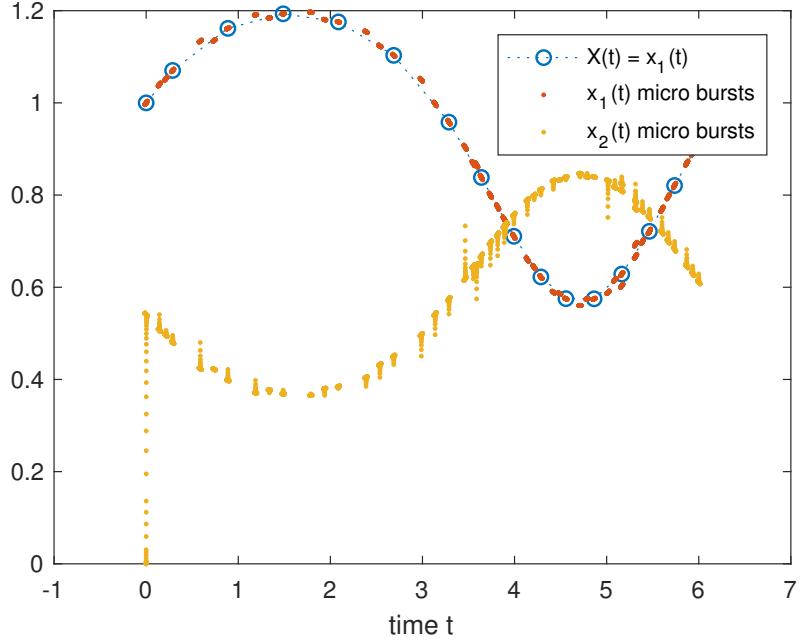
If the `cdmcFlag` is to be set without using a `restrict()` or `lift()` function, then use empty matrices `[]` for the restrict and lift functions.

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 i th 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(...)`

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



- `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

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

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

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

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

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

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

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

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

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

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

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

Plot output of this projective integration.

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

Upon finishing execution of the example, exit this function.

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

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

Section contents

2.5.1 Introduction	21
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2.5.1 Introduction

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

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

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

If no arguments, then execute an example

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

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

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

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

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

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

```
15 function [ts, xs] = MMburst(ti, xi, bT)
16     global MMepsilon
17     dMMdt = @(t,x) [ -x(1)+(x(1)+0.5)*x(2)
18                     1/MMepsilon*( x(1)-(x(1)+1)*x(2) ) ];
19     if ~exist('OCTAVE_VERSION','builtin')
20         [ts, xs] = ode23(dMMdt, [ti ti+bT], xi);
21     else % octave version
22         [ts, xs] = odeOct(dMMdt, [ti ti+bT], xi);
23     end
24 end

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

2.6 `cdmc()`: constraint defined manifold computing

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

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

Input

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

Output

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

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

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

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

3 Patch scheme for given microscale discrete space system

Chapter contents

3.1	<code>configPatches1()</code> : configures spatial patches in 1D	28
3.1.1	If no arguments, then execute an example	31
3.2	<code>patchSys1()</code> : interface 1D space to time integrators	34
3.3	<code>patchEdgeInt1()</code> : sets patch-edge values from interpolation over the 1D macroscale	35
3.4	<code>homogenisationExample</code> : simulate heterogeneous diffusion in 1D	37
3.4.1	Script to simulate via stiff or projective integration . .	38
3.4.2	<code>heteroDiff()</code> : heterogeneous diffusion	40
3.4.3	<code>heteroBurst()</code> : a burst of heterogeneous diffusion . .	41
3.5	<code>homoDiffEdgy1</code> : computational homogenisation of a 1D heterogeneous diffusion by simulation on small patches	42
3.5.1	Script code to simulate heterogeneous diffusion systems	42
3.5.2	<code>heteroDiff()</code> : heterogeneous diffusion	46
3.6	<code>Eckhardt2210eg2</code> : example of a 1D heterogeneous diffusion by simulation on small patches	48
3.6.1	Simulate heterogeneous diffusion systems	49
3.6.2	<code>heteroDiffF()</code> : forced heterogeneous diffusion . . .	51
3.7	<code>EckhardtEquilib</code> : find an equilibrium of a 1D heterogeneous diffusion via small patches	52
3.8	<code>EckhardtEquilibErrs</code> : explore errors in equilibria of a 1D heterogeneous diffusion on small patches	54
3.9	<code>Eckhardt2210eg1</code> : example of 1D space-time heterogeneous diffusion via computational homogenisation with projective integration and small patches	59
3.9.1	Simulate heterogeneous diffusion systems	60
3.9.2	<code>heteroBurstF()</code> : a burst of heterogeneous diffusion .	62
3.10	<code>homoLanLif1D</code> : computational homogenisation of a 1D heterogeneous Landau–Lifshitz by simulation on small patches . . .	63
3.10.1	Script code to simulate heterogeneous diffusion systems	64

3.10.2	Spectrum of the coded patch system	66
3.10.3	<code>heteroLanLif1D()</code> : heterogeneous Landau–Lifshitz PDE	68
3.11	<code>quasiLogAxes()</code> : transforms plot to quasi-log axes	69
3.12	<code>theRes()</code> : wrapper function to zero for equilibria	70
3.13	<code>configPatches2()</code> : configures spatial patches in 2D	71
3.13.1	If no arguments, then execute an example	74
3.14	<code>patchSys2()</code> : interface 2D space to time integrators	78
3.15	<code>patchEdgeInt2()</code> : sets 2D patch edge values from 2D macroscale interpolation	79
3.16	<code>monoscaleDiffEquil2</code> : equilibrium of a 2D monoscale heterogeneous diffusion via small patches	81
3.16.1	<code>monoscaleDiffForce2()</code> : microscale discretisation inside patches of forced diffusion PDE	83
3.17	<code>twoscaleDiffEquil2</code> : equilibrium of a 2D twoscale heterogeneous diffusion via small patches	84
3.17.1	<code>twoscaleDiffForce2()</code> : microscale discretisation inside patches of forced diffusion PDE	86
3.18	<code>twoscaleDiffEquil2Errs</code> : errors in equilibria of a 2D twoscale heterogeneous diffusion via small patches	87
3.18.1	<code>twoscaleDiffForce2()</code> : microscale discretisation inside patches of forced diffusion PDE	92
3.19	<code>abdulleDiffEquil2</code> : equilibrium of a 2D multiscale heterogeneous diffusion via small patches	94
3.19.1	<code>abdulleDiffForce2()</code> : microscale discretisation inside patches of forced diffusion PDE	96
3.20	<code>randAdvecDiffEquil2</code> : equilibrium of a 2D random heterogeneous advection-diffusion via small patches	97
3.20.1	<code>randAdvecDiffForce2()</code> : microscale discretisation inside patches of forced diffusion PDE	99
3.21	<code>homoWaveEdgy2</code> : computational homogenisation of a forced, non-autonomous, 2D wave via simulation on small patches	101
3.21.1	<code>heteroWave2()</code> : heterogeneous Waves	104
3.22	<code>configPatches3()</code> : configures spatial patches in 3D	106
3.22.1	If no arguments, then execute an example	110
3.22.2	<code>heteroWave3()</code> : heterogeneous Waves	112
3.23	<code>patchSys3()</code> : interface 3D space to time integrators	114

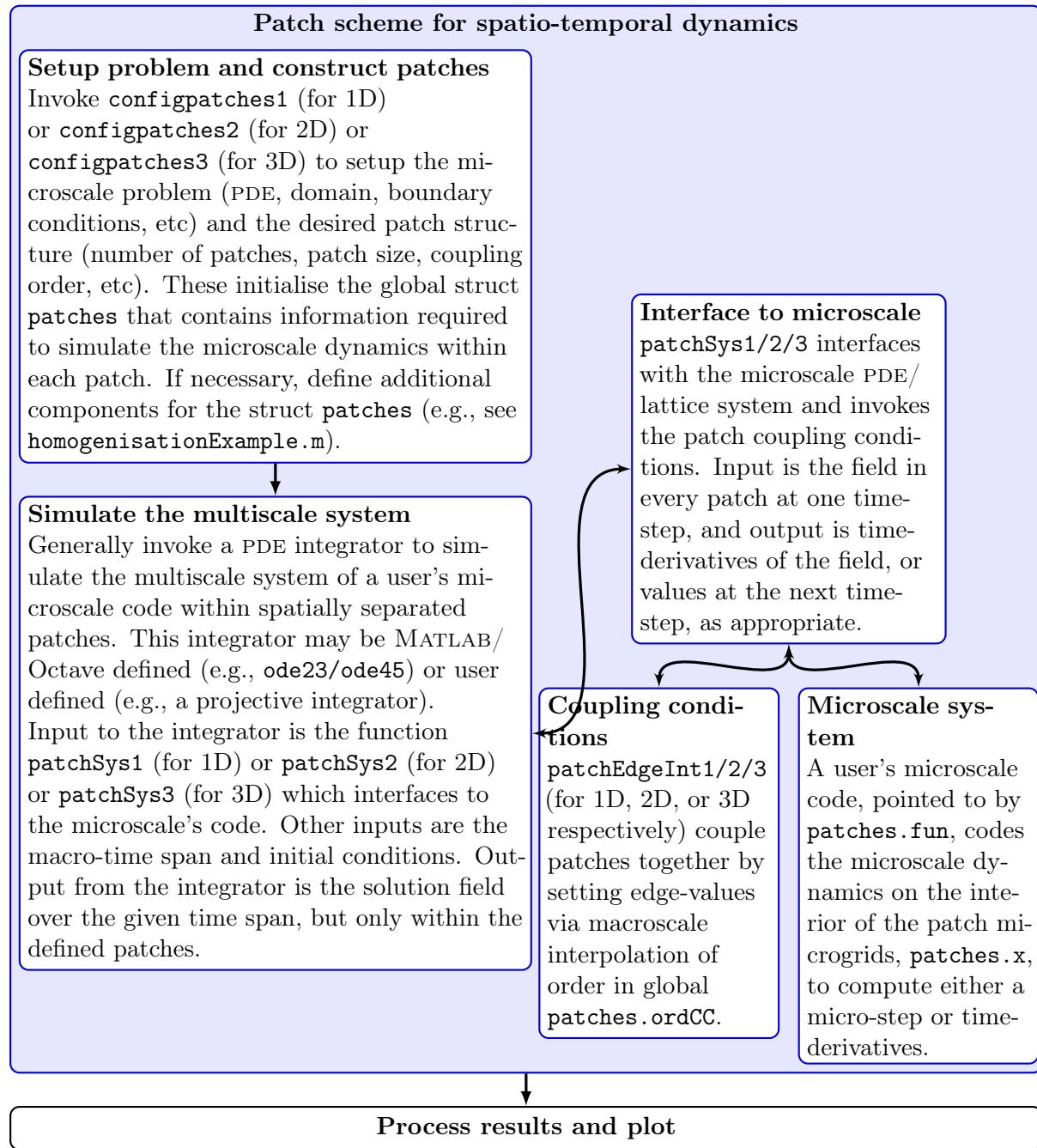
3.24 <code>patchEdgeInt3()</code> : sets 3D patch face values from 3D macroscale interpolation	116
3.25 <code>homoDiffEdgy3</code> : computational homogenisation of a 3D diffusion via simulation on small patches	118
3.25.1 Simulate heterogeneous diffusion	118
3.25.2 Compute Jacobian and its spectrum	120
3.25.3 <code>heteroDiff3()</code> : heterogeneous diffusion	122
3.26 <code>homoDiffBdryEqui13</code> : equilibrium via computational homogenisation of a 3D heterogeneous diffusion on small patches	124
3.26.1 <code>microDiffBdry3()</code> : 3D forced heterogeneous diffusion with boundaries	126

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).

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

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



3.1 configPatches1(): configures spatial patches in 1D

Section contents

3.1.1 If no arguments, then execute an example 31

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

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

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)`, 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. So either $\text{ratio} = \frac{1}{2}$ 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 must be odd so that there is a centre-patch lattice point.
- `nEdge` (not yet implemented), *optional*, default=1, for each patch, 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.
 - 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

- ```
180 if nargout==0, global patches, end
```
- `.fun` is the name of the user’s function `fun(t,u,patches)` or `fun(t,u)`, 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×1×1×nPatch` array of the regular spatial locations  $x_{iI}$  of the  $i$ th microscale grid point in the  $I$ th patch.
  - `.ratio`, only for macro-periodic conditions, is the size ratio of every patch.
  - `.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

---

<sup>1</sup> 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,  $(n_{\text{SubP}}(1) - 1) \times n_c$  2D array of microscale heterogeneous coefficients, or
- if `nEnsem` > 1,  $(n_{\text{SubP}}(1) - 1) \times n_c \times m_x$  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

```
252 if nargin==0
253 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 (" $\leftrightarrow$ " denotes function recursion).

1. `configPatches1`
2. `ode15s` integrator  $\leftrightarrow$  `patchSys1`  $\leftrightarrow$  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  $2\pi$ -periodic domain, with eight patches, spectral interpolation couples the patches, with micro-grid spacing 0.06, and with seven microscale points forming each patch.

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

Set some initial condition, with some microscale randomness.

```
280 u0=0.3*(1+sin(patches.x))+0.1*randn(size(patches.x));
```

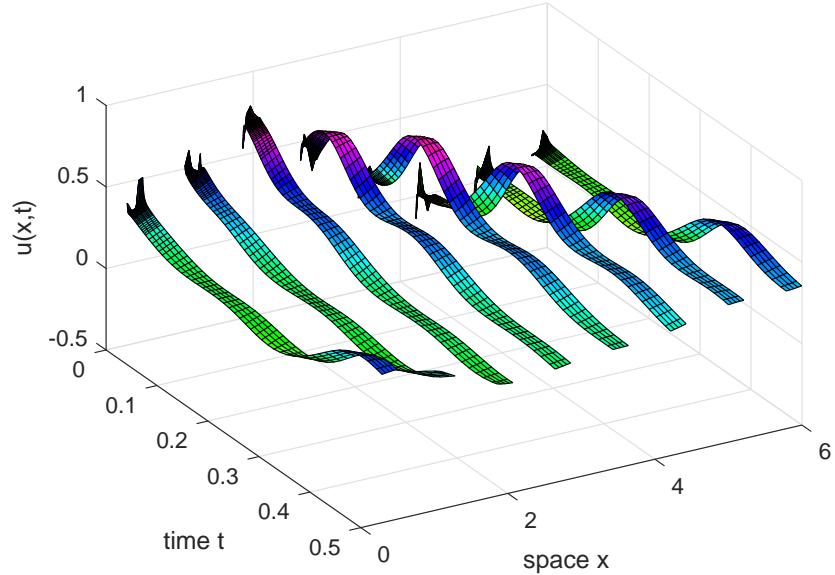
Simulate in time using a standard stiff integrator and the interface function `patchSys1()` ([Section 3.2](#)).

```
288 if ~exist('OCTAVE_VERSION','builtin')
289 [ts,us] = ode15s(@patchSys1, [0 0.5], u0(:));
290 else % octave version
291 [ts,us] = ode0cts(@patchSys1, [0 0.5], u0(:));
292 end
```

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.

```
304 figure(1),clf
305 if 1, patches.x([1 end],:,:, :)=nan; us=us.';
306 else us=reshape(patchEdgyInt1(us.'),[],length(ts));
```

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



```

307 end
308 surf(ts,patches.x(:,us)
309 view(60,40), colormap(0.8* hsv)
310 title('Burgers PDE: patches in space, continuous time')
311 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.

```

325 if OurCf2eps(mfilename)
326 return
327 end%if nargin==0

```

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

```

15 function ut=BurgersPDE(t,u,patches)
16 u=squeeze(u); % omit singleton dimensions
17 dx=diff(patches.x(1:2)); % microscale spacing
18 i=2:size(u,1)-1; % interior points in patches
19 ut=nan+u; % preallocate output array
20 ut(i,:)=diff(u,2)/dx^2 ...
21 -30*u(i,:).* (u(i+1,:)-u(i-1,:))/(2*dx);
22 end
23
24
25 function [ts,xs] = ode0cts(dxdt,tSpan,x0)
26 if length(tSpan)>2, ts = tSpan;

```

```
12 else ts = linspace(tSpan(1),tSpan(end),21)';
13 end
14 lsode_options('integration method','non-stiff');
15 xs = lsode(@(x,t) dxdt(t,x),x0,ts);
16 end
```

### 3.2 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. It mostly assumes that the sub-patch structure is *smooth enough* so that the patch centre-values are sensible macroscale variables, and patch edge values are determined by macroscale interpolation of the patch-centre or edge values. Nonetheless, microscale heterogeneous systems may be accurately simulated with this function via appropriate interpolation. Communicate patch-design variables ([Section 3.1](#)) either via the global struct `patches` or via an optional third argument (except that this last is required for parallel computing of `spmd`).

```
28 function dudt=patchSys1(t,u,patches)
29 if nargin<3, global patches, end
```

#### Input

- `u` is a vector/array of length  $n_{SubP} \cdot n_{Vars} \cdot n_{Ensem} \cdot n_{Patch}$  where there are  $n_{Vars} \cdot n_{Ensem}$  field values at each of the points in the  $n_{SubP} \times n_{Patch}$  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  $n_{SubP} \times n_{Vars} \times n_{Ensem} \times n_{Patch}$ . Time derivatives should be computed into the same sized array, then herein the patch edge values are overwritten by zeros.
  - `.x` is  $n_{SubP} \times 1 \times 1 \times n_{Patch}$  array of the spatial locations  $x_i$  of the microscale grid points in every patch. Currently it *must* be an equi-spaced lattice on both macro- and microscales.

#### Output

- `dudt` is a vector/array of time derivatives, but with patch edge-values set to zero. It is of total length  $n_{SubP} \cdot n_{Vars} \cdot n_{Ensem} \cdot n_{Patch}$  and the same dimensions as `u`.

### 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). <sup>2</sup>

Communicate patch-design variables via a second argument (optional, except required for parallel computing of spmd), or otherwise via the global struct patches.

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

#### Input

- **u** is a vector/array of length  $n_{SubP} \cdot n_{Vars} \cdot n_{Ensem} \cdot n_{Patch}$  where there are  $n_{Vars} \cdot n_{Ensem}$  field values at each of the points in the  $n_{SubP} \times n_{Patch}$  multiscale spatial grid.
- **patches** a struct largely set by configPatches1(), and which includes the following.
  - **.x** is  $n_{SubP} \times 1 \times 1 \times n_{Patch}$  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  $\geq -1$ .
  - **.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).
  - **.nEnsem** the number of realisations in the ensemble.

---

<sup>2</sup> Script patchEdgeInt1test.m verifies this code.

- `.parallel` whether serial or parallel.
- `.nCore`<sup>3</sup>

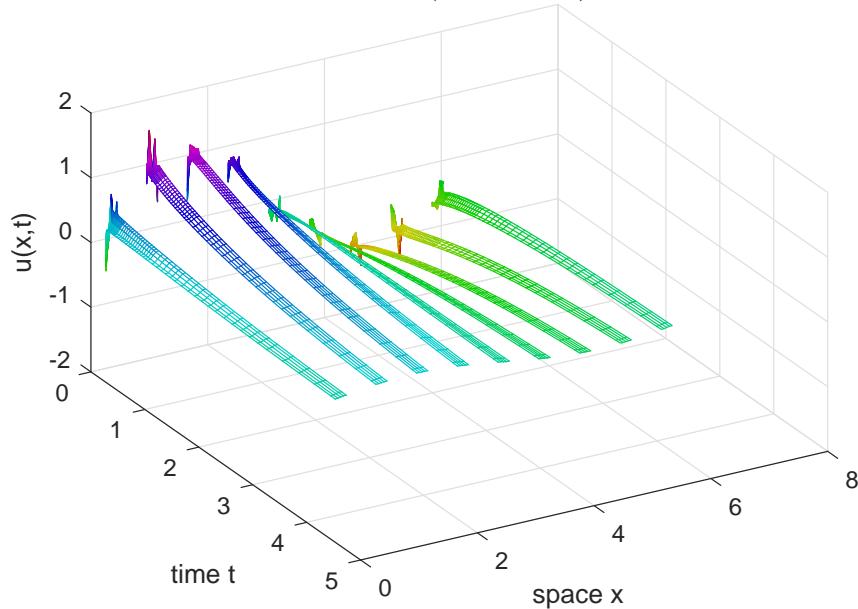
## Output

- `u` is 4D array, `nSubP × nVars × nEnsem × nPatch`, of the fields with edge values set by interpolation.

---

<sup>3</sup> **ToDo:** introduced sometime but not fully implemented yet, because prefer ensemble

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

|       |                                                                           |    |
|-------|---------------------------------------------------------------------------|----|
| 3.4.1 | Script to simulate via stiff or projective integration . . . . .          | 38 |
| 3.4.2 | <code>heteroDiff()</code> : heterogeneous diffusion . . . . .             | 40 |
| 3.4.3 | <code>heteroBurst()</code> : a burst of heterogeneous diffusion . . . . . | 41 |

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`  $\leftrightarrow$  `patchSys1`  $\leftrightarrow$  `heteroDiff`
3. process results

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

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

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

### 3.4.1 Script to simulate via stiff or projective integration

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

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

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

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

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

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

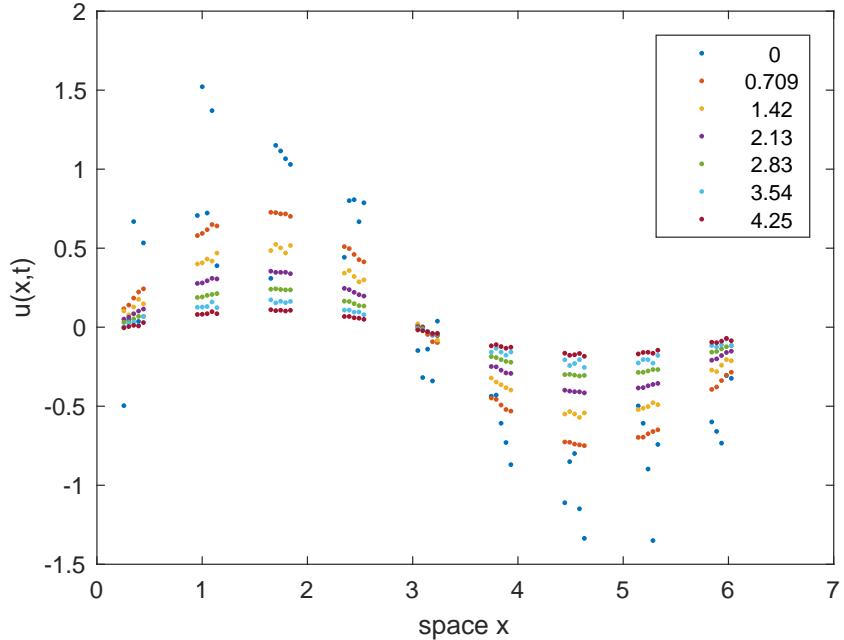
Plot the simulation in [Figure 3.3](#).

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

The code may invoke this integration interface.

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

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



```

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

```

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

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

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

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

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

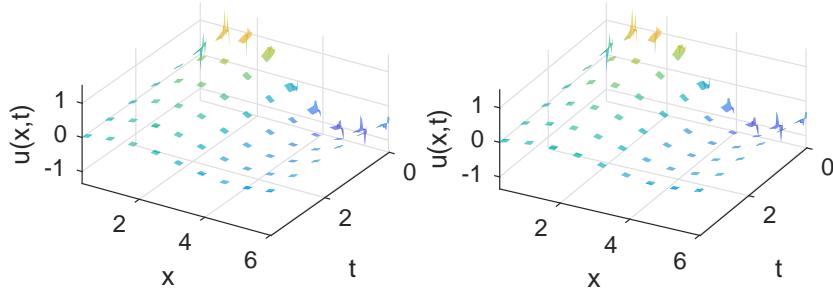
Set the desired macro- and microscale time-steps over the time domain: the macroscale step is in proportion to the effective mean diffusion time on the macroscale; the burst time is proportional to the intra-patch effective diffusion time; and lastly, the microscale time-step is proportional to the diffusion time between adjacent points in the microscale lattice.

```

153 ts = linspace(0,2/cHomo,7)
154 bT = 3*(ratio*Len/nPatch)^2/cHomo

```

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.



```

155 addpath('..../ProjInt')
156 [us,tss,uss] = PIRK2(@heteroBurst, ts, u0(:), bT);

```

Plot the macroscale predictions to draw Figure 3.4.

```

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

```

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

```

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

```

End of this example script.

### 3.4.2 heteroDiff(): heterogeneous diffusion

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

```

21 function ut = heteroDiff(t,u,patches)
22 dx = diff(patches.x(2:3)); % space step
23 i = 2:size(u,1)-1; % interior points in a patch
24 ut = nan+u; % preallocate output array
25 ut(i,:,:,:) = diff(patches.cs(:,1,:).*diff(u))/dx^2;
26 % possibly include heterogeneous Burgers' advection
27 if size(patches.cs,2)>1 % check for advection coeffs

```

---

```

28 buu = patches.cs(:,2,:).*u.^2;
29 ut(i,:) = ut(i,:)-(buu(i+1,:)-buu(i-1,:))/(dx*2);
30 end
31 end% function

```

### 3.4.3 heteroBurst(): a burst of heterogeneous diffusion

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

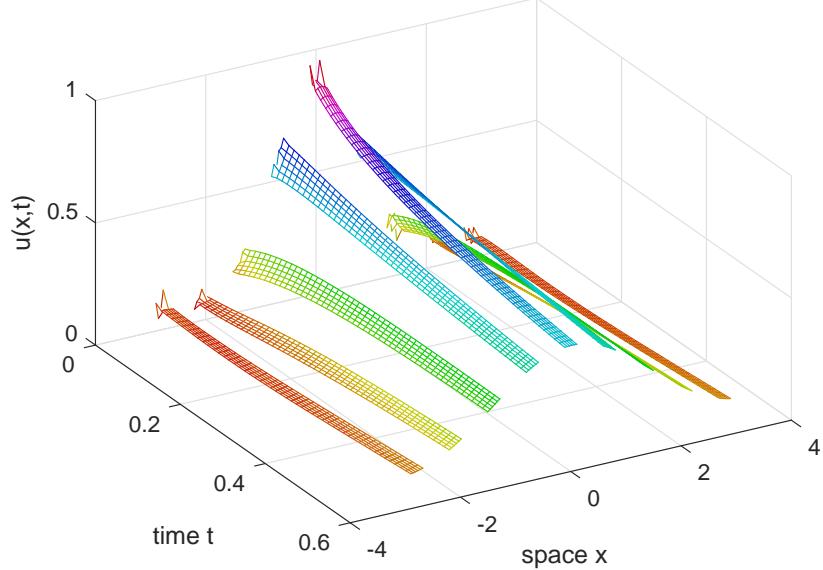
```

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

```

Fin.

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



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

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

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

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

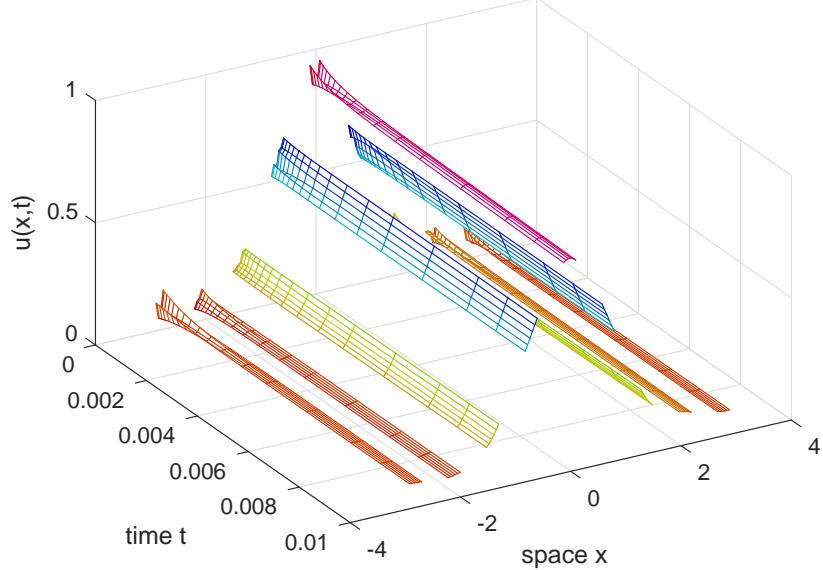
in terms of the centred difference operator  $\delta$ . The system has a microscale heterogeneity via the coefficients  $c_{i+1/2}$  which we assume to have some given known periodicity. Figure 3.6 shows one patch simulation of this system: observe the effects of the heterogeneity within each patch.

#### 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  $\leftrightarrow$  patchSys1  $\leftrightarrow$  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  $2\pi$  should have near integer decay rates, the squares of  $0, 1, 2, \dots$ . Then the heterogeneity is repeated to fill each patch, and phase-shifted for an ensemble.

```

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

```

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

```

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

```

```

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

```

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

```

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

```

Integrate using standard integrators.

```

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

```

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

```

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

```

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

```

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

```

```

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

```

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

```

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

```

Form the Jacobian matrix, linear operator, by numerical construction about a zero field. Use  $i$  to store the indices of the micro-grid points that are interior to the patches and hence are the system variables.

```

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

```

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

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

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

```

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

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

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

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

End of the main script.

```

### 3.5.2 `heteroDiff()`: heterogeneous diffusion

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

```

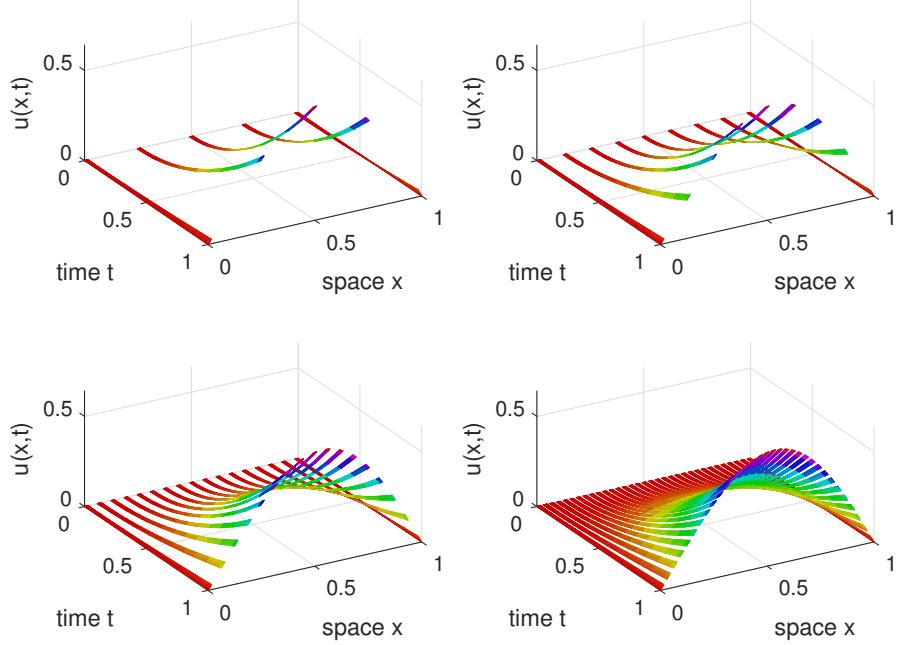
21 function ut = heteroDiff(t,u,patches)
22 dx = diff(patches.x(2:3)); % space step
23 i = 2:size(u,1)-1; % interior points in a patch

```

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

Fin.

Figure 3.8: diffusion field  $u(x, t)$  of the patch scheme applied to the forced heterogeneous diffusive (3.3). Simulate for 5, 9, 17, 33 patches and compare to the full-domain simulation (65 patches, not shown).



### 3.6 Eckhardt2210eg2: example of a 1D heterogeneous diffusion by simulation on small patches

Plot an example simulation in time generated by the patch scheme applied to macroscale forced diffusion through a medium with microscale heterogeneity in space. This is more-or-less the second example of [Eckhardt & Verfürth \(2022\)](#) [§6.2.1].

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

$$\frac{\partial u_i}{\partial t} = \frac{1}{dx^2} \delta[a_{i+1/2} \delta u_i] + f_i(t), \quad (3.3)$$

in terms of the centred difference operator  $\delta$ . The system has a microscale heterogeneity via the coefficients  $a_{i+1/2}$  which has some given known periodicity  $\epsilon$ .

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 3.8](#). 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).

### 3.6.1 Simulate heterogeneous diffusion systems

First establish the microscale heterogeneity has micro-period `mPeriod` on the lattice, and coefficients to match Eckhardt2210.04536 §6.2.1. Set the phase of the heterogeneity so that each patch centre is a point of symmetry of the diffusivity. Then the heterogeneity is repeated to fill each patch.

```

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

```

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

```

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

```

Loop to explore errors on various sized patches.

```

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

```

Determine indices of patches that are common in various resolutions

```

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

```

Establish the global data struct `patches` for the microscale heterogeneous lattice diffusion system (3.3) solved on domain [0, 1], with `nP` patches, and say fourth order interpolation to provide the edge-values. Setting `patches.EdgeyInt` true means the edge-values come from interpolating the opposite next-to-edge values of the patches (not the mid-patch values).

```

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

```

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

```

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

```

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

```

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

```

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

```

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

```

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

```

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

```

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

```

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

```

```

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

```

### 3.6.2 heteroDiffF(): forced heterogeneous diffusion

This function codes the lattice heterogeneous diffusion inside the patches with forcing and with microscale boundary conditions on the macroscale boundaries. Computes the time derivative at each point in the interior of a patch, output in `ut`. The column vector of diffusivities  $a_i$  has been stored in struct `patches.cs`, as has the array of forcing coefficients.

```
17 function ut = heteroDiffF(t,u,patches)
```

Cater for the two cases: one of a non-autonomous forcing oscillating in time when `microTimePeriod > 0`, or otherwise the case of an autonomous diffusion constant in time.

```

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

```

Two basic parameters, and initialise result array to NaNs.

```

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

```

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

```

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

```

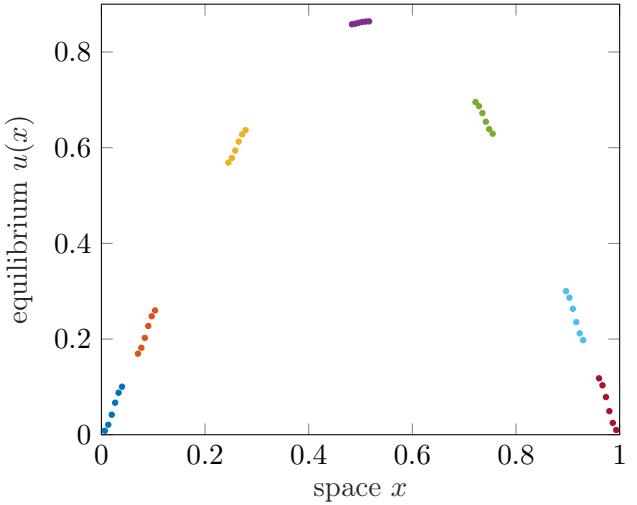
Code the microscale forced diffusion.

```

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

```

*Figure 3.9: 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.*



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

Sections 3.6 and 3.6.2 describe details of the problem and more details of the following configuration. The aim is to find the equilibrium, Figure 3.9, 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 3.9.

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

```

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

```

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

```

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

```

Establish the global data struct `patches` for the microscale heterogeneous lattice diffusion system (3.3) solved on domain  $[0, 1]$ , with Chebyshev-like distribution of patches, and say fourth order interpolation to provide the

edge-values. Use ‘edgy’ interpolation.

```
77 ordCC = 4
78 configPatches1(@heteroDiffF,[0 1], 'chebyshev', nPatch ...
79 ,ordCC,dx,nSubP,'EdgyInt',true,'hetCoeffs',a);
```

Set the forcing coefficients, either the original parabolic, or exp-sinusoidal. At time  $t = 1$  the resultant forcing we actually apply here is simply the sum of the two components.

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

**Find equilibrium with fsolve** We seek the equilibrium for the forcing that applies at time  $t = 1$  (as if that specific forcing were applying for all time). For this linear problem, it is computationally quicker using a linear solver, but **fsolve** is quicker in human time, Start the search from a zero field.

```
107 u = 0*patches.x;
```

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

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

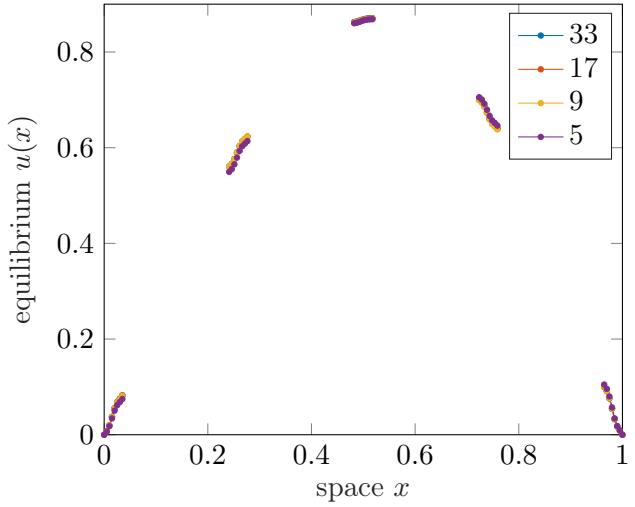
Seek the equilibrium, and report the norm of the residual, via the generic patch system wrapper `theRes` ([Section 3.12](#)).

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

**Plot the equilibrium** see [Figure 3.9](#).

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

*Figure 3.10:* 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.



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

Section 3.7 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 3.10 and 3.11. Find mean-abs errors to be the following:

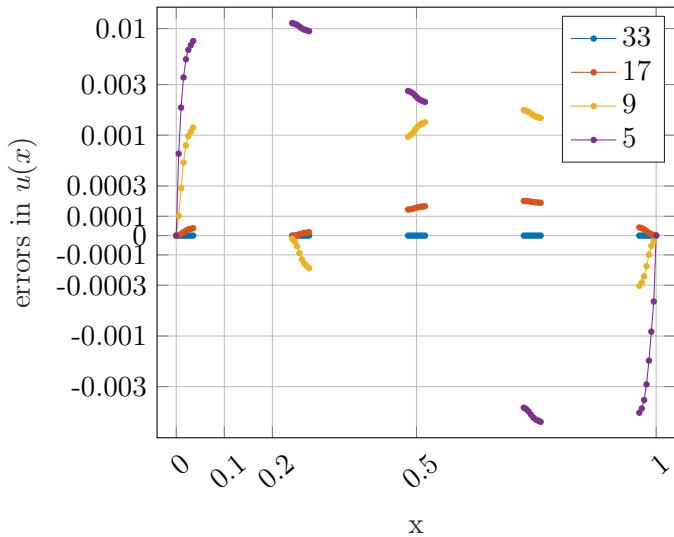
|           | $N =$        | 5    | 9    | 17   | 33   | 65    |
|-----------|--------------|------|------|------|------|-------|
| equispace | second-order | 8E-3 | 1E-2 | 1E-2 | 4E-3 | 9E-4  |
| equispace | fourth-order | 2E-3 | 7E-4 | 1E-4 | 9E-6 | 5E-7  |
| equispace | sixth-order  | 2E-3 | 2E-5 | 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’<sup>4</sup>. 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

<sup>4</sup> But the error assessment is with respect to finest patch-grid, no longer with a full domain solution

*Figure 3.11: Errors in the equilibrium of the heterogeneous diffusion problem for relatively large  $\epsilon = 0.03$ . The solution is obtained with various numbers of patches, but we only plot the errors within these five common patches.*



different (despite the magnitude of the solution being a little larger).

|           | $N =$        | 5    | 9    | 17   | 33   | 65   |
|-----------|--------------|------|------|------|------|------|
| equispace | fourth-order | 4E-3 | 7E-4 | 1E-4 | 8E-6 | 5E-7 |
| chebyshev | fourth-order | 7E-4 | 2E-3 | 5E-4 | 3E-4 | 1E-4 |
| usergiven | fourth-order | 2E-3 | 3E-3 | 5E-4 | 4E-5 | 2E-6 |

Clear, and initiate global patches. Choose the type of patch distribution to be either 'equispace', 'chebyshev', or 'usergiven'. Also set order of interpolation (fourth-order is good start).

```

136 clear all
137 global patches
138 %global OurCf2eps, OurCf2eps=true %option to save plots
139 switch 1
140 case 1, Dom.type = 'equispace'
141 case 2, Dom.type = 'chebyshev'
142 case 3, Dom.type = 'usergiven'
143 end% switch
144 ordInt = 4

```

**First configure the patch system** Establish the microscale heterogeneity has micro-period `mPeriod` on the lattice, and coefficients to match Eckhardt2210.04536 §6.2.1.

```

155 mPeriod = 6
156 z = (0.5:mPeriod)'/mPeriod;
157 a = 1./(2-cos(2*pi*z))
158 global microTimePeriod; microTimePeriod=0;

```

To use a hierarchy of patches with `nPatch` of 5, 9, 17, ..., we need up to  $N$  patches plus one `dx` to fit into the domain interval. Cater for up to some full-domain simulation—can compute  $\log 2N_{\max} = 129$  ( $\epsilon = 0.008$ ) in a few seconds:

```

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

Set the periodicity ϵ , and other microscale parameters.

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

```

**For various numbers of patches** Choose five to be the coarsest number of patches. Want place to store common results for the solutions. Assign Ps to be the indices of the common patches: for equispace set to the five common patches, but for chebyshev the only common ones are the three centre and boundary-adjacent patches.

```

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

```

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

```
205 nPatch = 2^log2N+1
```

In the case of ‘usergiven’, we choose standard Chebyshev distribution of the centre of the patches, which involves overlapping of patches near the boundaries! (instead of the coded chebyshev which has a boundary layer of non-overlapping patches and a Chebyshev within the interior).

```

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

```

Configure the patches:

```

226 configPatches1(@heteroDiffF,[0 1],Dom,nPatch ...
227 ,ordInt,dx,nSubP,'EdgyInt',true,'hetCoeffs',a);

```

Set the forcing coefficients, either the original parabolic, or sinusoidal. At time  $t = 1$  the resultant forcing we actually apply here is simply the sum of the two components.

```

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

```

```

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

```

**Solve for steady state** Set initial guess of either zero or a subsample of the next finer solution, with NaN to indicate patch-edge values. Index  $i$  are the indices of patch-interior points, and the number of unknowns is then its length.

```

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

```

Solve via `fsolve` for simplicity and robustness (and using `optimoptions` to omit trace information), via the generic patch system wrapper `theRes` ([Section 3.12](#)).

```

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

```

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

```

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

```

Concatenate the solution on common patches into stores.

```

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

```

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

```

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

```

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

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

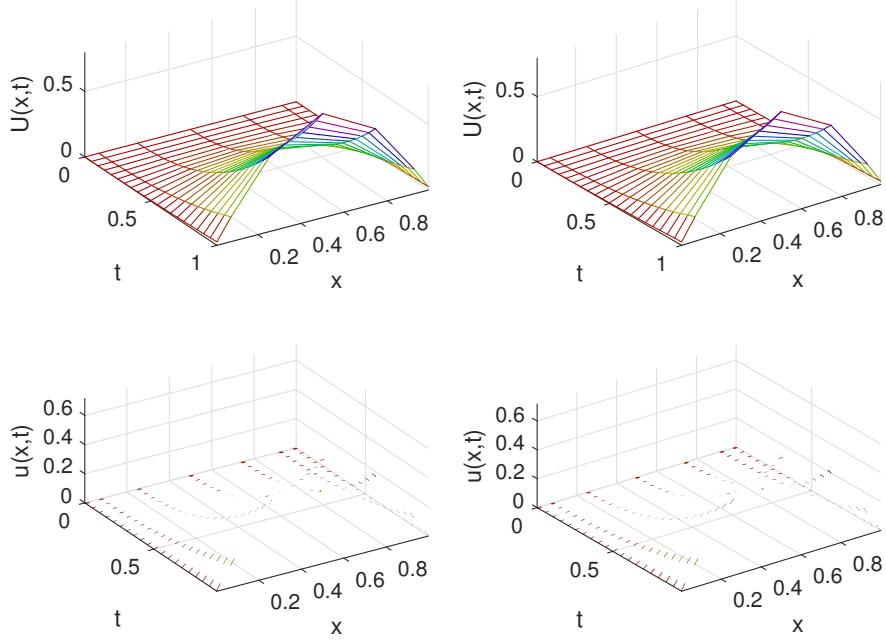
 Reshape solution field.

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

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

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

*Figure 3.12: diffusion field  $u(x, t)$  of the patch scheme applied to the forced space-time heterogeneous diffusive (3.4). 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.*



### 3.9 Eckhardt2210eg1: example of 1D space-time heterogeneous diffusion via computational homogenisation with projective integration and small patches

An example simulation in time generated by projective integration allied with the patch scheme applied to forced diffusion in a medium with microscale heterogeneity in both space and time. This is more-or-less the first example of [Eckhardt & Verfürth \(2022\)](#) [§6.2].

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

$$\frac{\partial u_i}{\partial t} = \frac{1}{dx^2} \delta[a_{i+1/2}(t) \delta u_i] + f_i(t), \quad (3.4)$$

in terms of the centred difference operator  $\delta$ . The system has a microscale heterogeneity via the coefficients  $a_{i+1/2}$  which has given periodicity  $\epsilon$  in space, and periodicity  $\epsilon^2$  in time. [Figure 3.12](#) 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’.

### 3.9.1 Simulate heterogeneous diffusion systems

First establish the microscale heterogeneity has micro-period `mPeriod` on the spatial lattice, and coefficients inspired by Eckhardt2210.04536 §6.2. Set the phase of the heterogeneity so that each patch centre is a point of symmetry of the diffusivity. Then the heterogeneity is repeated to fill each patch. If an odd number of odd-periods in a patch, then the centre patch is a grid point of the field  $u$ , otherwise the centre patch is at a half-grid point.

```

98 clear all
99 %global OurCf2eps, OurCf2eps=true %option to save plots
100 mPeriod = 6
101 y = linspace(0,1,mPeriod+1)';
102 a = (3+cos(2*pi*y(1:mPeriod)))/30
103 A0 = 1/mean(1./a) % roughly the effective diffusivity

```

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

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

```

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

```

Set the time periodicity (global).

```

126 global microTimePeriod
127 microTimePeriod = 1/rEpsilon^2

```

Establish the global data struct `patches` for the microscale heterogeneous lattice diffusion system (3.4) solved on macroscale domain  $[0, 1]$ , with `nPatch` patches, and say fourth-order interpolation to provide the edge-values of the inter-patch coupling conditions. Distribute the patches either equispaced or chebyshev. Setting `patches.EdgyInt` true means the edge-values come from interpolating the opposite next-to-edge values of the patches (not the mid-patch values).

```

144 nPatch = 7
145 ordCC = 4

```

```

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

```

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

```

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

```

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

```

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

```

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

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

```

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

```

Time the projective integration simulation.

```

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

```

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

```

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

```

```

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

```

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

```

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

```

### 3.9.2 heteroBurstF(): a burst of heterogeneous diffusion

This code integrates in time the derivatives computed by `heteroDiff` from within the patch coupling of `patchSys1`. Try `ode23`, although `ode45` may give smoother results. Sample every period of the microscale time fluctuations (or, at least, close to the period).

```

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

```

### 3.10 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  $\alpha$ , we explore the dynamics of  $\vec{M}(x, t)$  governed by the nonlinear Landau–Lifshitz PDE (Leitenmaier & Runborg 2021, (1.1))<sup>5</sup>

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

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

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

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

in terms of the centred difference operator  $\delta$ . 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 3.13](#) 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  $\alpha$  should be small. If the initial conditions are smooth, then `ode15s` has no problems for  $\alpha = 0.001$ .<sup>6</sup>

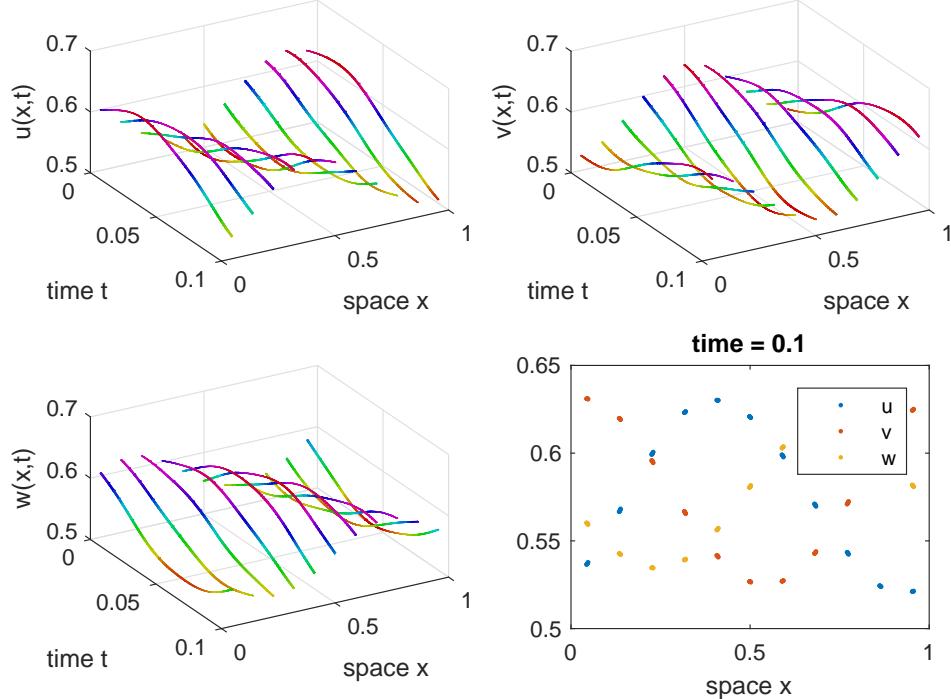
```
89 global alpha ex5p1
90 ex5p1 = 0; % set to 1 for L&O example of p.27
91 alpha = 0.001 % phenomenological damping parameter
```

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

<sup>5</sup> Recall  $a \times (b \times c) = (a \cdot c)b - (a \cdot b)c$

<sup>6</sup> 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 3.13: magnetic field  $\vec{M}(x, t) = (u, v, w)$  of the gap-tooth scheme applied to the heterogeneous Landau–Lifshitz PDE to show the emergent macroscale wave-like dynamics. This simulation uses eleven patches in space of size ratio 0.055. Compare the time  $t = 0.1$  graph with Fig. 2.1 of [Leitenmaier & Runborg \(2021\)](#).



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

### 3.10.1 Script code to simulate heterogeneous diffusion systems

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

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

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

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

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

values).

```

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

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

```

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

Integrate using standard integrators.

```

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

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

```

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

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

```

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

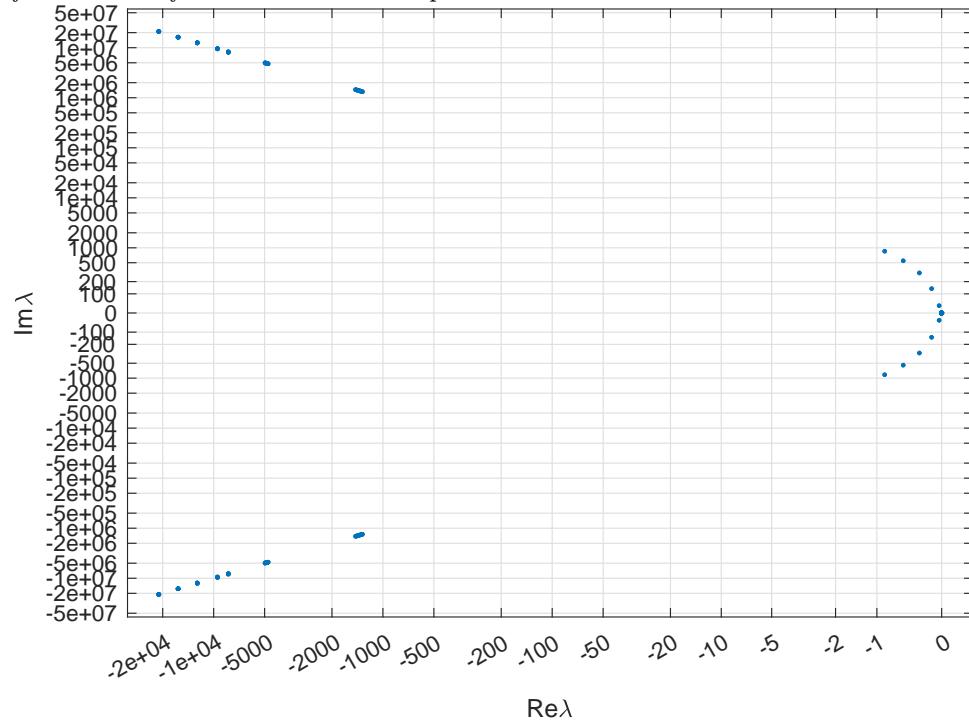
**Plot space-time surface of the simulation** Choose whether to save some plots, or not.

```

208 global OurCf2eps
209 OurCf2eps = false;
```

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

Figure 3.14: spectrum of eigenvalues of the multiscale patch scheme applied to the Landau–Lifshitz PDE. The macroscale eigenvalues are clearly separated from those of the microscale sub-patch modes.



```

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

```

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

```

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

```

### 3.10.2 Spectrum of the coded patch system

It appears the spectrum has the following properties as shown by [Figure 3.14](#), with  $N = \text{nPatch}$  and  $n = \text{nSubP} - 2$ , and on base of  $\vec{M} = \vec{1}/\sqrt{3}$ .

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

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

```

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

```

Form the Jacobian by numerical differentiation.

```

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

```

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

```

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

```

Plot the spectrum of eigenvalues on quasi-log axes.

```

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

```

### 3.10.3 `heteroLanLif1D()`: heterogeneous Landau–Lifshitz PDE

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

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

```

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

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

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

```

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

```

47 i = 2:size(M,1)-1; % interior points in a patch
48 MH=nan+H; % preallocate for MxH
49 MH(:,3,:,:)= M(i,1,:,:).*H(:,2,:,:)-M(i,2,:,:).*H(:,1,:,:);
50 MH(:,2,:,:)= M(i,3,:,:).*H(:,1,:,:)-M(i,1,:,:).*H(:,3,:,:);
51 MH(:,1,:,:)= M(i,2,:,:).*H(:,3,:,:)-M(i,3,:,:).*H(:,2,:,:);
52 MMH=nan+H; % preallocate for MxMxH
53 MMH(:,3,:,:)= M(i,1,:,:).*MH(:,2,:,:)-M(i,2,:,:).*MH(:,1,:,:);
54 MMH(:,2,:,:)= M(i,3,:,:).*MH(:,1,:,:)-M(i,1,:,:).*MH(:,3,:,:);
55 MMH(:,1,:,:)= M(i,2,:,:).*MH(:,3,:,:)-M(i,3,:,:).*MH(:,2,:,:);
56 Mt = nan+M; % preallocate output array
57 Mt(i,:,:,:)= -MH-alpha*MMH;
58 end% function

```

Fin.

### 3.11 quasiLogAxes(): transforms plot to quasi-log axes

This function rescales and labels the axes of the given 2D plot. The original aim was to effectively show the complex spectrum of multiscale systems such as the patch scheme. The eigenvalues are over a wide range of magnitudes, but are signed. So we use a nonlinear asinh transformation of the axes, and then label the axes with reasonable ticks. The nonlinear rescaling is useful in other scenarios also.

Herein  $x, y$  denotes the original data scale, and  $h, v$  denotes nonlinearly transformed quantities.

```
20 function quasiLogAxes(handle,xScale,yScale)
```

#### Input

- **handle**: handle to your plot to transform, for example, obtained by `handle=plot(...)`
- **xScale** (optional, default 1): let  $x$  denote every horizontal coordinate, then transform the plot-data with the `asinh()` function so that
  - for  $|x| \lesssim x_{\text{scale}}$  the horizontal axis scaling is approximately linear, whereas
  - for  $|x| \gtrsim x_{\text{scale}}$  the horizontal axis scaling is approximately signed-logarithmic.
- **yScale** (optional, default 1): corresponds to **xScale** for the vertical axis scaling.
- axis limits (optional): if the axis limits of the plot do not 'fit' the plot data, then we assume you have set the axis limits, in which case these limits are used (horizontal and vertical are considered separately).

**Example** If invoked with no arguments, then execute an example.

```
48 if nargin==0
49 % first generate your data
50 n=99; fast=(rand(n,1)<0.8);
51 z = -rand(n,1).*(1+1e3*fast)+1i*randn(n,1).*(5+1e2*fast);
52 % second plot data and transform axes
53 handle = plot(real(z),imag(z),'o');
54 xlabel('real-part'), ylabel('imag-part')
55 quasiLogAxes(handle,1,10);
56 return
57 end% example
```

Default values for scaling.

```
65 if nargin<3, yScale=1; end
66 if nargin<2, xScale=1; end
```

**Output** None, just the transformed plot.

### 3.12 theRes(): wrapper function to zero for equilibria

This functions converts a vector of values into the interior values of the patches, then evaluates the time derivative of the system at time  $t = 1$ , and returns the vector of patch-interior time derivatives.

```
15 function f=theRes(u)
16 global patches
17 switch numel(size(patches.x))
18 case 4, pSys = @patchSys1;
19 v=nan(size(patches.x));
20 case 5, pSys = @patchSys2;
21 v=nan(size(patches.x+patches.y));
22 case 6, pSys = @patchSys3;
23 v=nan(size(patches.x+patches.y+patches.z));
24 otherwise error('number of dimensions is somehow wrong')
25 end%switch
26 v(patches.i) = u;
27 f = pSys(1,v(:,),patches);
28 f = f(patches.i);
29 end%function theRes
```

### 3.13 configPatches2(): configures spatial patches in 2D

#### *Section contents*

##### 3.13.1 If no arguments, then execute an example . . . . . 74

Makes the struct `patches` for use by the patch/gap-tooth time derivative/step function `patchSys2()`. [Section 3.13.1](#) lists an example of its use.

```
19 function patches = configPatches2(fun,Xlim,Dom ...
20 ,nPatch,ordCC,dx,nSubP,varargin)
```

**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 3.13.1](#) for an example code.

- `fun` is the name of the user function, `fun(t,u,patches)` or `fun(t,u)`, that computes time-derivatives (or time-steps) of quantities on the 2D micro-grid within all the 2D patches.
- `Xlim` array/vector giving the rectangular macro-space domain of the computation, namely  $[Xlim(1), Xlim(2)] \times [Xlim(3), Xlim(4)]$ . If `Xlim` has two elements, then the domain is the square domain of the same interval in both directions.
- `Dom` sets the type of macroscale conditions for the patches, and reflects the type of microscale boundary conditions of the problem. If `Dom` is `NaN` or `[]`, then the field `u` is doubly macro-periodic in the 2D spatial domain, and resolved on equi-spaced patches. If `Dom` is a character string, then that specifies the `.type` of the following structure, with `.bcOffset` set to the default zero. Otherwise `Dom` is a structure with the following components.
  - `.type`, string, of either `'periodic'` (the default), `'equispace'`, `'chebyshev'`, `'usergiven'`. For all cases except `'periodic'`, users *must* code into `fun` the micro-grid boundary conditions that apply at the left/right/bottom/top edges of the leftmost/rightmost/bottommost/topmost patches, respectively.
  - `.bcOffset`, optional one, two or four element vector/array, in the cases of `'equispace'` or `'chebyshev'` the patches are placed so the left/right/top/bottom macroscale boundaries are aligned to the left/right/top/bottom edges of the corresponding extreme patches, but offset by `.bcOffset` of the sub-patch micro-grid spacing. For example, use `bcOffset=0` when the micro-code applies Dirichlet boundary values on the extreme edge micro-grid points, whereas use `bcOffset=0.5` when the microcode applies Neumann boundary conditions halfway between the extreme edge micro-grid points. Similarly for the top and bottom edges.

If `.bcOffset` is a scalar, then apply the same offset to all boundaries. If two elements, then apply the first offset to both  $x$ -boundaries, and the second offset to both  $y$ -boundaries. If four elements, then apply the first two offsets to the respective  $x$ -boundaries, and the last two offsets to the respective  $y$ -boundaries.

- `.X`, optional vector/array with `nPatch(1)` elements, in the case '`usergiven`' it specifies the  $x$ -locations of the centres of the patches—the user is responsible the locations makes sense.
- `.Y`, optional vector/array with `nPatch(2)` elements, in the case '`usergiven`' it specifies the  $y$ -locations of the centres of the patches—the user is responsible the locations makes sense.
- `nPatch` sets the number of equi-spaced spatial patches: if scalar, then use the same number of patches in both directions, otherwise `nPatch(1:2)` gives the number of patches ( $\geq 1$ ) in each direction.
- `ordCC` is the ‘order’ of interpolation for inter-patch coupling across empty space of the macroscale patch values to the edge-values of the patches: currently must be 0, 2, 4, . . . ; where 0 gives spectral interpolation.
- `dx` (real—scalar or two element) is usually the sub-patch micro-grid spacing in  $x$  and  $y$ . If scalar, then use the same `dx` in both directions, otherwise `dx(1:2)` gives the spacing in each of the two directions.

However, if `Dom` is `NaN` (as for pre-2023), then `dx` actually is `ratio` (scalar or two element), namely the ratio of (depending upon `EdgyInt`) either the half-width or full-width of a patch to the equi-spacing of the patch mid-points. So either `ratio = ½` means the patches abut and `ratio = 1` is overlapping patches as in holistic discretisation, or `ratio = 1` means the patches abut. Small `ratio` should greatly reduce computational time.

- `nSubP` is the number of equi-spaced microscale lattice points in each patch: if scalar, then use the same number in both directions, otherwise `nSubP(1:2)` gives the number in each direction. If not using `EdgyInt`, then must be odd so that there is/are centre-patch micro-grid point/lines in each patch.
- `nEdge` (not yet implemented), *optional*, default=1, for each patch, 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/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.
  - 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.<sup>7</sup>

- ```
206 if nargout==0, global patches, end
```
- **.fun** is the name of the user's function **fun(t,u,patches)** or **fun(t,u)**, 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.

⁷ When using **spmd** parallel computing, it is generally best to avoid global variables, and so instead prefer using an explicit output variable.

- `.stag` is true for interpolation using only odd neighbouring patches as for staggered grids, and false for the usual case of all neighbour coupling—not yet implemented.
- `.Cwtsr` and `.Cwts1`, only for macro-periodic conditions, are the `ordCC` \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 \times 2, only for macro-periodic conditions, are the size ratios of every patch.
- `.nEdge` is, for each patch, the number of edge values set by interpolation at the edge regions of each patch.
- `.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.

3.13.1 If no arguments, then execute an example

```
289 if nargin==0
290 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 (" \leftrightarrow " denotes function recursion).

1. configPatches2
2. ode23 integrator \leftrightarrow patchSys2 \leftrightarrow 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).

```
313 global patches
314 patches = configPatches2(@nonDiffPDE, [-3 3 -2 2], [] ...
315     , [9 7], 0, 0.12, 5 , 'EdgyInt', false);
```

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

```
322 u0 = exp(-patches.x.^2-patches.y.^2);
323 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.

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

Start by showing the initial conditions of [Figure 3.15](#) while the simulation computes.

```
340 u = reshape(permute(squeeze(u0) ...
341     ,[1 3 2 4]), [numel(x) numel(y)]);
342 hsurf = surf(x(:, ),y(:, ),u');
343 axis([-3 3 -3 3 -0.03 1]), view(60,40)
344 legend('time = 0.00','Location','north')
345 xlabel('space x'), ylabel('space y'), zlabel('u(x,y)')
346 colormap(hsv)
347 if0urCf2eps([mfilename 'ic'])
```

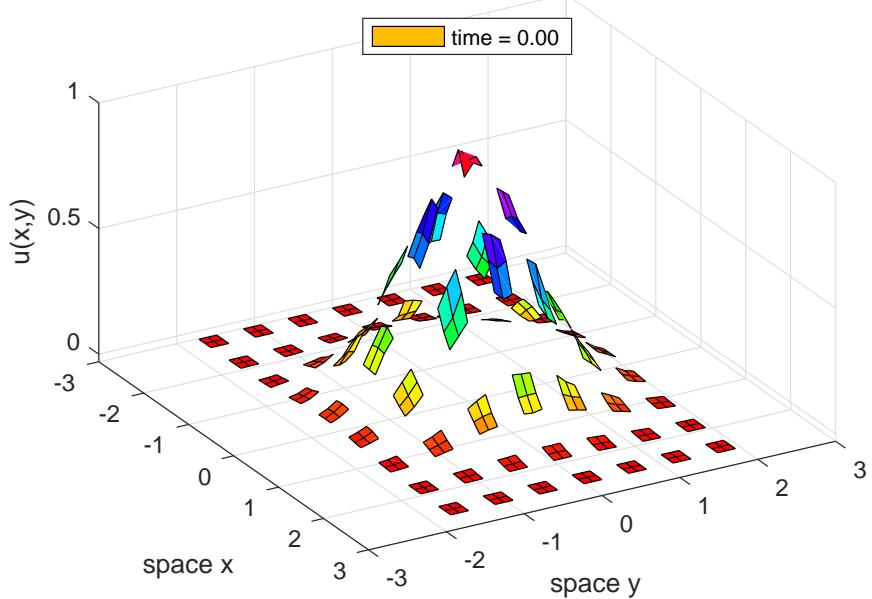
Integrate in time to $t = 4$ using standard functions. In MATLAB `ode15s` would be natural as the patch scheme is naturally stiff, but `ode23` is quicker ([Maclean et al. 2020](#), Fig. 4). Ask for output at non-uniform times because the diffusion slows.

```
364 disp('Wait to simulate nonlinear diffusion h_t=(h^3)_xx+(h^3)_yy')
365 drawnow
366 if ~exist('OCTAVE_VERSION','builtin')
367     [ts,us] = ode23(@patchSys2,linspace(0,2).^2,u0(:));
368 else % octave version is quite slow for me
369     lsode_options('absolute tolerance',1e-4);
370     lsode_options('relative tolerance',1e-4);
371     [ts,us] = odeOcts(@patchSys2,[0 1],u0(:));
372 end
```

Animate the computed simulation to end with [Figure 3.16](#). Use `patchEdgeInt2` to interpolate patch-edge values.

```
380 for i = 1:length(ts)
```

Figure 3.15: initial field $u(x, y, t)$ at time $t = 0$ of the patch scheme applied to a nonlinear ‘diffusion’ PDE: Figure 3.16 plots the computed field at time $t = 3$.



```

381     u = patchEdgeInt2(us(i,:));
382     u = reshape(permute(squeeze(u) ...
383             ,[1 3 2 4]), [numel(x) numel(y)]);
384     set(hsurf,'ZData', u');
385     legend(['time = ' num2str(ts(i),'%4.2f')]);
386     pause(0.1)
387 end
388 if0urCf2eps([mfilename 't3'])

```

Upon finishing execution of the example, exit this function.

```

403 return
404 end%if no arguments

```

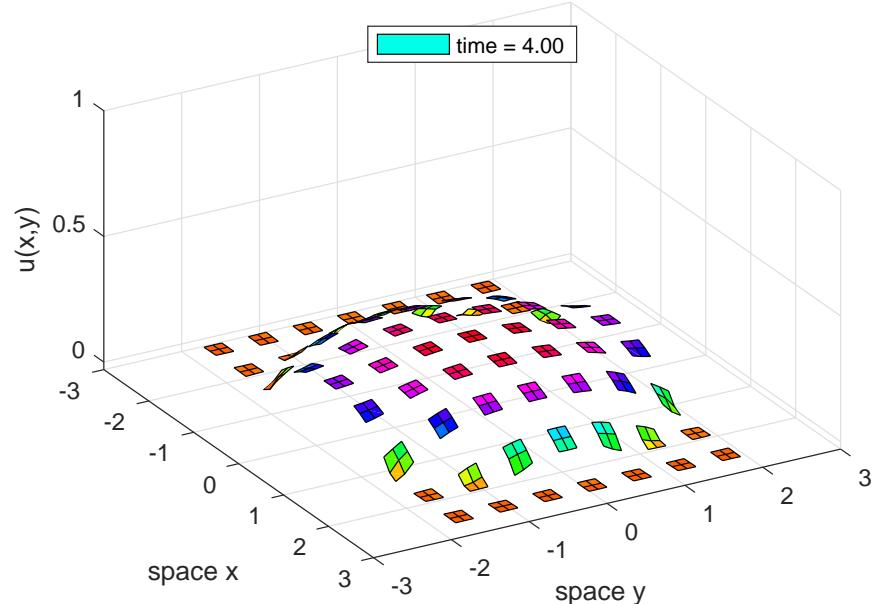
Example of nonlinear diffusion PDE inside patches As a microscale discretisation of $u_t = \nabla^2(u^3)$, code $\dot{u}_{ijkl} = \frac{1}{\delta x^2}(u_{i+1,j,k,l}^3 - 2u_{i,j,k,l}^3 + u_{i-1,j,k,l}^3) + \frac{1}{\delta y^2}(u_{i,j+1,k,l}^3 - 2u_{i,j,k,l}^3 + u_{i,j-1,k,l}^3)$.

```

13 function ut = nonDiffPDE(t,u,patches)
14     if nargin<3, global patches, end
15     u = squeeze(u); % reduce to 4D
16     dx = diff(patches.x(1:2)); % microgrid spacing
17     dy = diff(patches.y(1:2));
18     i = 2:size(u,1)-1; j = 2:size(u,2)-1; % interior patch points
19     ut = nan+u; % preallocate output array
20     ut(i,j,:,:,:) = diff(u(:,:,j,:,:).^3,2,1)/dx^2 ...
21                         +diff(u(:,:,i,:,:).^3,2,2)/dy^2;
22 end

```

Figure 3.16: field $u(x, y, t)$ at time $t = 3$ of the patch scheme applied to a nonlinear ‘diffusion’ PDE with initial condition in Figure 3.15.



3.14 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. It assumes that the sub-patch structure is *smooth enough* so that the patch centre-values are sensible macroscale variables, and patch edge-values are determined by macroscale interpolation of the patch-centre or edge values. Nonetheless, microscale heterogeneous systems may be accurately simulated with this function via appropriate interpolation. Communicate patch-design variables (Section 3.13) either via the global struct `patches` or via an optional third argument (except that this last is required for parallel computing of `spmd`).

```
28 function dudt = patchSys2(t,u,patches)
29 if nargin<3, global patches, end
```

Input

- `u` is a vector/array of length $\text{prod}(\text{nSubP}) \cdot \text{nVars} \cdot \text{nEnsem} \cdot \text{prod}(\text{nPatch})$ where there are `nVars` · `nEnsem` field values at each of the points in the `nSubP(1)` × `nSubP(2)` × `nPatch(1)` × `nPatch(2)` grid.
- `t` is the current time to be passed to the user's time derivative function.
- `patches` a struct set by `configPatches2()` with the following information used here.
 - `.fun` is the name of the user's function `fun(t,u,patches)` that computes the time derivatives on the patchy lattice. The array `u` has size `nSubP(1)` × `nSubP(2)` × `nVars` × `nEnsem` × `nPatch(1)` × `nPatch(2)`. Time derivatives must be computed into the same sized array, although herein the patch edge-values are overwritten by zeros.
 - `.x` is `nSubP(1)` × `1` × `1` × `1` × `nPatch(1)` × `1` array of the spatial locations x_i of the microscale (i, j) -grid points in every patch. Currently it *must* be an equi-spaced lattice on both macro- and micro-scales.
 - `.y` is similarly `1` × `nSubP(2)` × `1` × `1` × `1` × `nPatch(2)` array of the spatial locations y_j of the microscale (i, j) -grid points in every patch. Currently it *must* be an equi-spaced lattice on both macro- and micro-scales.

Output

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

3.15 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.⁸

Communicate patch-design variables via a second argument (optional, except required for parallel computing of spmd), or otherwise via the global struct patches.

```
29 function u = patchEdgeInt2(u,patches)
30 if nargin<2, global patches, end
```

Input

- `u` is a vector/array of length `prod(nSubP)·nVars·nEnsem·prod(nPatch)` where there are `nVars · nEnsem` field values at each of the points in the `nSubP1 · nSubP2 · nPatch1 · nPatch2` multiscale spatial grid on the `nPatch1 · nPatch2` array of patches.
- `patches` a struct set by configPatches2() which includes the following information.
 - `.x` is `nSubP1×1×1×1×nPatch1×1` array of the spatial locations x_{iI} of the microscale grid points in every patch. Currently it *must* be an equi-spaced lattice on the microscale index i , but may be variable spaced in macroscale index I .
 - `.y` is similarly $1 \times nSubP2 \times 1 \times 1 \times 1 \times nPatch2$ array of the spatial locations y_{jJ} of the microscale grid points in every patch. Currently it *must* be an equi-spaced lattice on the microscale index j , but may be variable spaced in macroscale index J .
 - `.ordCC` is order of interpolation, currently only $\{0, 2, 4, \dots\}$
 - `.periodic` indicates whether macroscale is periodic domain, or alternatively that the macroscale has left, right, top and bottom boundaries so interpolation is via divided differences.
 - `.stag` in $\{0, 1\}$ is one for staggered grid (alternating) interpolation. Currently must be zero.
 - `.Cwtsr` and `.Cwtsl` are the coupling coefficients for finite width interpolation in both the x, y -directions—when invoking a periodic domain.
 - `.EdgyInt`, true/false, for determining patch-edge values by interpolation: true, from opposite-edge next-to-edge values (often

⁸ Script `patchEdgeInt2test.m` verifies this code.

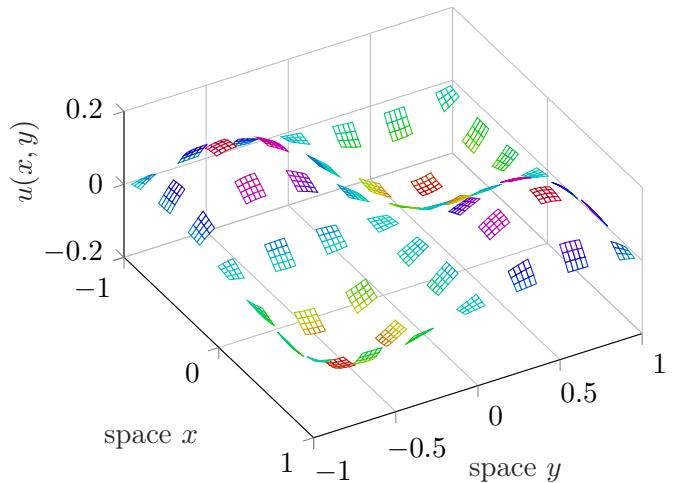
preserves symmetry); false, from centre cross-patch values (near original scheme).

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

Output

- `u` is 6D array, $n_{SubP1} \cdot n_{SubP2} \cdot n_{Vars} \cdot n_{Ensem} \cdot n_{Patch1} \cdot n_{Patch2}$, of the fields with edge values set by interpolation.

Figure 3.17:
Equilibrium of the macroscale diffusion problem of Freese with Dirichlet zero-value boundary conditions (Section 3.16). The patch size is not small so we can see the patches.



3.16 monoscaleDiffEquil2: equilibrium of a 2D monoscale heterogeneous diffusion via small patches

Here we find the steady state $u(x, y)$, see Figure 3.17, to the heterogeneous PDE (inspired by Freese et al.⁹ §5.2)

$$u_t = A(x, y) \vec{\nabla} \vec{\nabla} u - f,$$

on domain $[-1, 1]^2$ with Dirichlet BCs, for coefficient pseudo-diffusion matrix

$$A := \begin{bmatrix} 2 & a \\ a & 2 \end{bmatrix} \quad \text{with } a := \text{sign}(xy) \text{ or } a := \sin(\pi x) \sin(\pi y),$$

and for forcing $f(x, y)$ such that the exact equilibrium is $u = x(1 - e^{1-|x|})y(1 - e^{1-|y|})$. But for simplicity, let's obtain $u = x(1 - x^2)y(1 - y^2)$ for which we code f later—as determined by this Reduce algebra code.

```
on gcd; factor sin;
u:=x*(1-x^2)*y*(1-y^2);
a:=sin(pi*x)*sin(pi*y);
f:=2*df(u,x,x)+2*a*df(u,x,y)+2*df(u,y,y);
```

Clear, and initiate globals.

```
57 clear all
58 global patches
59 %global OurCf2eps, OurCf2eps=true %option to save plot
```

Patch configuration Initially use 7×7 patches in the square $(-1, 1)^2$. For continuous forcing we may have small patches of any reasonable microgrid spacing—here the microgrid error dominates.

⁹ <http://arxiv.org/abs/2211.13731>

```

70 nPatch = 7
71 nSubP = 5
72 dx = 0.03

Specify some order of interpolation.

78 configPatches2(@monoscaleDiffForce2,[-1 1 -1 1],'equispace' ...
79 ,nPatch ,4 ,dx ,nSubP ,'EdgyInt',true );

```

Compute the time-constant coefficient and time-constant forcing, and store them in struct `patches` for access by the microcode of [Section 3.16.1](#).

```

87 x=patches.x; y=patches.y;
88 patches.A = sin(pi*x).*sin(pi*y);
89 patches.fu = ...
90     +2*patches.A.*((9*x.^2.*y.^2-3*x.^2-3*y.^2+1) ...
91     +12*x.*y.*((x.^2+y.^2-2));

```

By construction, the PDE has analytic solution

```
97 uAnal = x.*((1-x.^2).*y.*((1-y.^2));
```

Solve for steady state Set initial guess of zero, with NaN to indicate patch-edge values. Index `i` are the indices of patch-interior points, and the number of unknowns is then its length.

```

110 u0 = zeros(nSubP,nSubP,1,1,nPatch,nPatch);
111 u0([1 end],:,:) = nan; u0(:,[1 end],:) = nan;
112 patches.i = find(~isnan(u0));
113 nVariables = numel(patches.i)

```

Solve by iteration. Use `fsolve` for simplicity and robustness (using `optimoptions` to omit its trace information), and give magnitudes.

```

121 tic;
122 uSoln = fsolve(@theRes,u0(patches.i) ...
123     ,optimoptions('fsolve','Display','off'));
124 solnTime = toc
125 normResidual = norm(theRes(uSoln))
126 normSoln = norm(uSoln)
127 normError = norm(uSoln-uAnal(patches.i))

```

Store the solution vector into the patches, and interpolate, but have not bothered to set boundary values so they stay NaN from the interpolation.

```

135 u0(patches.i) = uSoln;
136 u0 = patchEdgeInt2(u0);

```

Draw solution profile Separate patches with NaNs, then reshape arrays to suit 2D space surface plots.

```

147 figure(1), clf, colormap(0.8* hsv)
148 x(end+1,:,:)=nan; u0(end+1,:,:)=nan;

```

```

149 y(:,end+1,:)=nan; u0(:,end+1,:)=nan;
150 u = reshape(permute(squeeze(u0),[1 3 2 4]), [numel(x) numel(y)]);
Draw the patch solution surface, with boundary-values omitted as already NaN
by not bothering to set them.

157 mesh(x(:,y(:,u'));
158 xlabel('space $x$'), ylabel('space $y$'), zlabel('$u(x,y)$')
159 if0urCf2tex(mfilename)%optionally save

```

3.16.1 monoscaleDiffForce2(): microscale discretisation inside patches of forced diffusion PDE

This function codes the lattice heterogeneous diffusion of the PDE inside the patches. For 6D input arrays u , x , and y , computes the time derivative at each point in the interior of a patch, output in ut .

```

176 function ut = monoscaleDiffForce2(t,u,patches)
177 dx = diff(patches.x(2:3)); % x space step
178 dy = diff(patches.y(2:3)); % y space step
179 i = 2:size(u,1)-1; % x interior points in a patch
180 j = 2:size(u,2)-1; % y interior points in a patch
181 ut = nan+u; % preallocate output array

```

Set Dirichlet boundary value of zero around the square domain.

```

188 u( 1 ,:,:, :, 1 ,:) = 0; % left edge of left patches
189 u(end,:,:,:,end,:) = 0; % right edge of right patches
190 u(:, 1 ,:,:, :, 1 ) = 0; % bottom edge of bottom patches
191 u(:,end,:,:, :,end) = 0; % top edge of top patches

```

Or code some function variation around the boundary, such as a function of y on the left boundary, and a (constant) function of x at the top boundary.

```

199 if 0
200 u(1,:,:,:,1,:)=(1+patches.y)/2; % left edge of left patches
201 u(:,end,:,:, :,end)=1; % top edge of top patches
202 end%if

```

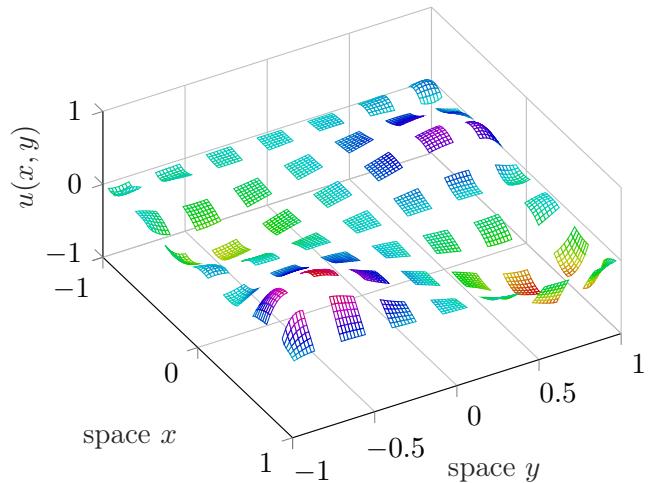
Compute the time derivatives via stored forcing and coefficients. Easier to code by conflating the last four dimensions into the one $,:$.

```

210 ut(i,j,:)
211 = 2*diff(u(:,j,:),2,1)/dx^2 +2*diff(u(i,:,:),2,2)/dy^2 ...
212 +2*patches.A(i,j,:).*( u(i+1,j+1,:)-u(i-1,j+1,:)) ...
213 -u(i+1,j-1,:)+u(i-1,j-1,:))/(4*dx*dy) ...
214 -patches.fu(i,j,:);
215 end%function monoscaleDiffForce2

```

Figure 3.18:
Equilibrium of the multiscale diffusion problem of Freese with Dirichlet zero-value boundary conditions (Section 3.17). 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.



3.17 twoscaleDiffEquil2: equilibrium of a 2D two-scale heterogeneous diffusion via small patches

Here we find the steady state $u(x, y)$ to the heterogeneous PDE (inspired by Freese et al.¹⁰ §5.3.1)

$$u_t = A(x, y) \vec{\nabla} \vec{\nabla} u - f,$$

on domain $[-1, 1]^2$ with Dirichlet BCs, for coefficient ‘diffusion’ matrix, varying with period 2ϵ on the microscale $\epsilon = 2^{-7}$, of

$$A := \begin{bmatrix} 2 & a \\ a & 2 \end{bmatrix} \quad \text{with } a := \sin(\pi x/\epsilon) \sin(\pi y/\epsilon),$$

and for forcing $f := (x + \cos 3\pi x)y^3$.

Clear, and initiate globals.

```
41 clear all
42 global patches
43 %global OurCf2eps, OurCf2eps=true %option to save plot
```

First establish the microscale heterogeneity has micro-period `mPeriod` on the spatial lattice. Set the phase of the heterogeneity so that each patch centre is a point of symmetry of the diffusivity. Then `configPatches2` replicates the heterogeneity to fill each patch.

```
56 mPeriod = 6
57 z = (0.5:mPeriod)'/mPeriod;
58 A = sin(2*pi*z).*sin(2*pi*z');
```

Set the periodicity, via ϵ , and other microscale parameters.

```
65 nPeriodsPatch = 1 % any integer
66 epsilon = 2^(-6) % 4 or 5 to see the patches
67 dx = (2*epsilon)/mPeriod
68 nSubP = nPeriodsPatch*mPeriod+2 % for edgy int
```

¹⁰ <http://arxiv.org/abs/2211.13731>

Patch configuration Say use 7×7 patches in $(-1, 1)^2$, fourth order interpolation, and either ‘equispace’ or ‘chebyshev’:

```
79 nPatch = 7
80 configPatches2(@twoscaleDiffForce2, [-1 1], 'equispace' ...
81 ,nPatch ,4 ,dx ,nSubP , 'EdgyInt',true , 'hetCoeffs',A );
```

Compute the time-constant forcing, and store in struct `patches` for access by the microcode of [Section 3.18.1](#).

```
89 x = patches.x; y = patches.y;
90 patches.fu = 100*(x+cos(3*pi*x)).*y.^3;
```

Solve for steady state Set initial guess of zero, with NaN to indicate patch-edge values. Index `i` are the indices of patch-interior points, and the number of unknowns is then its length.

```
104 u0 = zeros(nSubP,nSubP,1,1,nPatch,nPatch);
105 u0([1 end],:,:) = nan; u0(:,[1 end],:) = nan;
106 patches.i = find(~isnan(u0));
107 nVariables = numel(patches.i)
```

Solve by iteration. Use `fsolve` for simplicity and robustness (and using `optimoptions` to omit trace information), via the generic patch system wrapper `theRes` ([Section 3.12](#)), and give magnitudes.

```
116 tic;
117 uSoln = fsolve(@theRes,u0(patches.i) ...
118 ,optimoptions('fsolve','Display','off'));
119 solveTime = toc
120 normResidual = norm(theRes(uSoln))
121 normSoln = norm(uSoln)
```

Store the solution vector into the patches, and interpolate, but have not bothered to set boundary values so they stay NaN from the interpolation.

```
129 u0(patches.i) = uSoln;
130 u0 = patchEdgeInt2(u0);
```

Draw solution profile Separate patches with NaNs, then reshape arrays to suit 2D space surface plots.

```
141 figure(1), clf, colormap(0.8* hsv)
142 x(end+1,:,:)=nan; u0(end+1,:,:)=nan;
143 y(:,end+1,:)=nan; u0(:,end+1,:)=nan;
144 u = reshape(permute(squeeze(u0),[1 3 2 4]), [numel(x) numel(y)]);
```

Draw the patch solution surface, with boundary-values omitted as already NaN by not bothering to set them.

```
151 mesh(x(:,y(:,u')); view(60,55)
152 xlabel('space $x$'), ylabel('space $y$'), zlabel('$u(x,y)$')
153 ifOurCf2tex(mfilename)%optionally save
```

3.17.1 twoscaleDiffForce2(): microscale discretisation inside patches of forced diffusion PDE

This function codes the lattice heterogeneous diffusion of the PDE inside the patches. For 6D input arrays u , x , and y , computes the time derivative at each point in the interior of a patch, output in ut .

```

172  function ut = twoscaleDiffForce2(t,u,patches)
173      dx = diff(patches.x(2:3)); % x space step
174      dy = diff(patches.y(2:3)); % y space step
175      i = 2:size(u,1)-1; % x interior points in a patch
176      j = 2:size(u,2)-1; % y interior points in a patch
177      ut = nan+u;           % preallocate output array

```

Set Dirichlet boundary value of zero around the square domain.

```

184  u( 1 ,:,:, :, 1 ,:) = 0; % left edge of left patches
185  u(end,:,:,:,end,:) = 0; % right edge of right patches
186  u(:, 1 ,:,:, :, 1 ) = 0; % bottom edge of bottom patches
187  u(:,end,:,:, :,end) = 0; % top edge of top patches

```

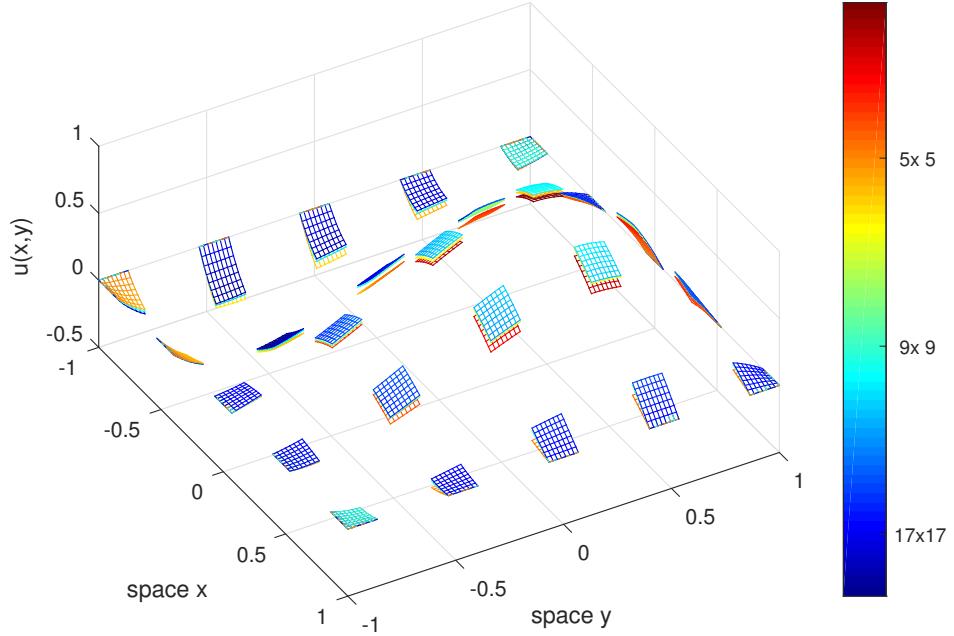
Compute the time derivatives via stored forcing and coefficients. Easier to code by conflating the last four dimensions into the one $,:$.

```

195  ut(i,j,:) ...
196  = 2*diff(u(:,j,:),2,1)/dx^2 +2*diff(u(:,j),2,2)/dy^2 ...
197  +2*patches.cs(i,j).*( u(i+1,j+1,:)-u(i-1,j+1,:)) ...
198  -(u(i+1,j-1,:)+u(i-1,j-1,:))/(4*dx*dy) ...
199  -patches.fu(i,j,:);
200 end%function twoscaleDiffForce2

```

Figure 3.19: 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 3.18). We only compare solutions only in these 25 common patches.



3.18 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

$$A := \begin{bmatrix} 2 & a \\ a & 2 \end{bmatrix} \quad \text{with } a := \sin(\pi x/\epsilon) \sin(\pi y/\epsilon),$$

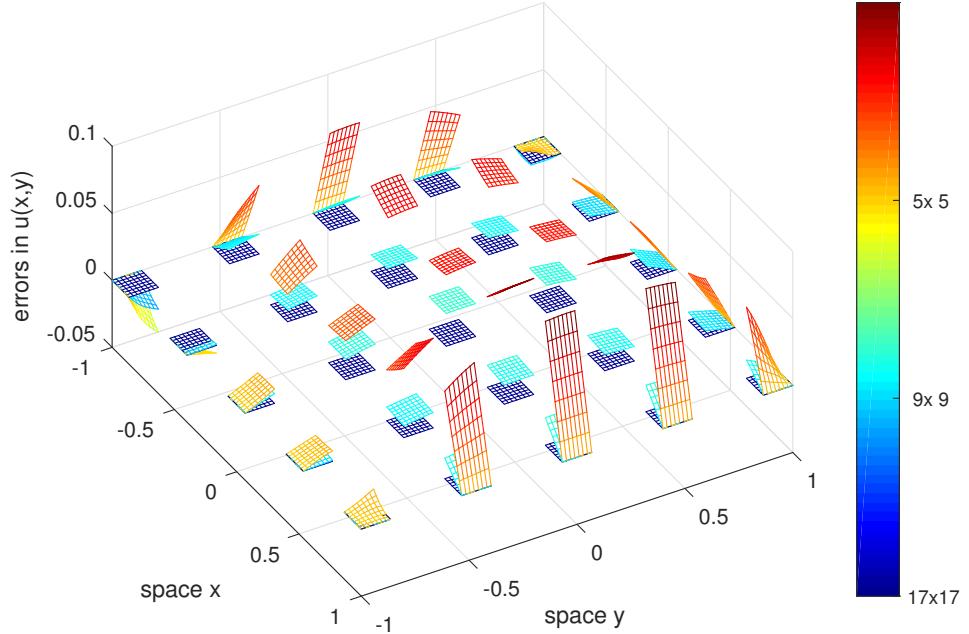
and for forcing $f := 10(x + y + \cos \pi x)$ (for which the solution has magnitude up to one).¹²

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 3.20: 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 3.18). We only compare solutions only in these 25 common patches.



interpolation and patch distribution):

	N	5	9	17	33
equispace, 2nd-order	6E-2	3E-2	1E-2	3E-3	
equispace, 4th-order	3E-2	8E-3	7E-4	7E-5	
chebyshev, 4th-order	1E-2	2E-2	6E-3	2E-3	
usergiven, 4th-order	1E-2	2E-2	4E-3	n/a	
equispace, 6th-order	3E-2	1E-3	1E-4	2E-5	

Script start Clear, and initiate global patches. Choose the type of patch distribution to be either ‘equispace’, ‘chebyshev’, or ‘usergiven’. Also set order of interpolation (fourth-order is good start).

```

81 clear all
82 global patches
83 %global OurCf2eps, OurCf2eps=true %option to save plot
84 switch 1
85     case 1, Dom.type = 'equispace'
86     case 2, Dom.type = 'chebyshev'
87     case 3, Dom.type = 'usergiven'
88 end% switch
89 ordInt = 4

```

First configure the patch system Establish the microscale heterogeneity has micro-period `mPeriod` on the spatial lattice. Then `configPatches2` replicates the heterogeneity as needed to fill each patch.

```

100 mPeriod = 6
101 z = (0.5:mPeriod)'/mPeriod;
102 A = sin(2*pi*z).*sin(2*pi*z)';

```

To use a hierarchy of patches with `nPatch` of 5, 9, 17, ..., we need up to N patches plus one `dx` to fit into the domain interval. Cater for up to some full-domain simulation—can compute `log2Nmax = 5` ($\epsilon = 0.06$) within minutes:

```

112 log2Nmax = 4 % >2 up to 6 OKish
113 nPatchMax=2^log2Nmax+1

```

Set the periodicity ϵ , and other microscale parameters.

```

120 nPeriodsPatch = 1 % any integer
121 nSubP = nPeriodsPatch*mPeriod+2 % for edgy int
122 epsilon = 2/(nPatchMax*nPeriodsPatch+1/mPeriod)
123 dx = epsilon/mPeriod

```

For various numbers of patches Choose five patches to be the coarsest number of patches. Define variables to store common results for the solutions from differing patches. Assign `Ps` to be the indices of the common patches: for equispace set to the five common patches, but for ‘chebyshev’ the only common ones are the three centre and boundary-adjacent patches.

```

136 us=[]; xs=[]; ys=[]; nPs=[];
137 for log2N=log2Nmax:-1:2
138     if log2N==log2Nmax
139         Ps=linspace(1,nPatchMax ...
140             ,5-2*all(Dom.type=='chebyshev'))
141     else Ps=(Ps+1)/2
142 end

```

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

```
148 nPatch = 2^log2N+1
```

In the case of ‘usergiven’, we set the standard Chebyshev distribution of the patch-centres, which involves overlapping of patches near the boundaries! (instead of the coded chebyshev which has boundary layers of abutting patches, and non-overlapping Chebyshev between the boundary layers).

```

159 if all(Dom.type=='usergiven')
160     halfWidth = dx*(nSubP-1)/2;
161     X1 = -1+halfWidth; X2 = 1-halfWidth;
162     Dom.X = (X1+X2)/2-(X2-X1)/2*cos(linspace(0,pi,nPatch));
163     Dom.Y = Dom.X;
164 end

```

Configure the patches:

```

170 configPatches2(@twoscaleDiffForce2,[-1 1],Dom,nPatch ...
171     ,ordInt ,dx ,nSubP , 'EdgyInt',true , 'hetCoeffs',A );

```

Compute the time-constant forcing, and store in struct `patches` for access by the microcode of [Section 3.18.1](#).

```

179     if 1
180         patches.fu = 10*(patches.x+cos(pi*patches.x)+patches.y);
181     else patches.fu = 8+0*patches.x+0*patches.y;
182     end

```

Solve for steady state Set initial guess of either zero or a subsample of the previous, next-finer, solution. `NaN` indicates patch-edge values. Index `i` are the indices of patch-interior points, and the number of unknowns is then its length.

```

193     if log2N==log2Nmax
194         u0 = zeros(nSubP,nSubP,1,1,nPatch,nPatch);
195     else u0 = u0(:,:,(:,:,1:2:end,1:2:end));
196     end
197     u0([1 end],:,:) = nan; u0(:,[1 end],:) = nan;
198     patches.i = find(~isnan(u0));
199     nVariables = numel(patches.i)

```

First try to solve via iterative solver `bicgstab`, via the generic patch system wrapper `theRes` ([Section 3.12](#)).

```

207     tic;
208     maxIt = ceil(nVariables/10);
209     rhsb = theRes( zeros(size(patches.i)) );
210     [uSoln,flag] = bicgstab(@(u) rhsb-theRes(u),rhsb ...
211                             ,1e-9,maxIt,[],[],u0(patches.i));
212     bicgTime = toc

```

However, the above often fails (and `fsolve` sometimes takes too long here), so then try a preconditioned version of `bicgstab`. The preconditioner is derived from the Jacobian which is expensive to find (four minutes for $N = 33$, one hour for $N = 65$), but we do so as follows.

```

222     if flag>0, disp('**** bicg failed, trying ILU preconditioner')
223         disp(['Computing Jacobian: wait roughly ' ...
224               num2str(nPatch^4/4500,2) ' secs'])
225         tic
226         Jac=sparse(nVariables,nVariables);
227         for j=1:nVariables
228             Jac(:,j)=sparse( rhsb-theRes((1:nVariables)'==j) );
229         end
230         formJacTime=toc

```

Compute an incomplete LU -factorization, and use it as preconditioner to `bicgstab`.

```

237     tic
238     [L,U] = ilu(Jac,struct('type','ilutp','droptol',1e-4));
239     LUfillFactor = (nnz(L)+nnz(U))/nnz(Jac)

```

```

240      [uSoln,flag] = bicgstab(@(u) rhsb-theRes(u),rhsb ...
241                      ,1e-9,maxIt,L,U,u0(patches.i));
242      precondSolveTime=toc
243      assert(flag==0,'preconditioner fails bicgstab. Lower droptol?')
244 end%if flag

```

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

```

251      normResidual = norm(theRes(uSoln),Inf)
252      normSoln = norm(uSoln,Inf)
253      u0(patches.i) = uSoln;
254      u0 = patchEdgeInt2(u0);
255      u0( 1 ,:,:, :, 1 ,:) = 0; % left edge of left patches
256      u0(end,:,:, :,end,:) = 0; % right edge of right patches
257      u0(:, 1 ,:,:, :, 1 ) = 0; % bottom edge of bottom patches
258      u0(:,end,:,:, :,end) = 0; % top edge of top patches
259      assert(normResidual<1e-5,'poor--bad solution found')

```

Concatenate the solution on common patches into stores.

```

265      us=cat(5,us,squeeze(u0(:,:, :, :,Ps,Ps)));
266      xs=cat(3,xs,squeeze(patches.x(:,:, :, :,Ps,:)));
267      ys=cat(3,ys,squeeze(patches.y(:,:, :, :, :,Ps,:)));
268      nPs = [nP;nP];

```

End loop. Check micro-grids are aligned, then compute errors compared to the full-domain solution (or the highest resolution solution for the case of ‘usergiven’).

```

277 end%for log2N
278 assert(max(abs(reshape(diff(xs,1,3),[],1)))<1e-12,'x-coord failure')
279 assert(max(abs(reshape(diff(ys,1,3),[],1)))<1e-12,'y-coord failure')
280 errs = us-us(:,:, :, :,1);
281 meanAbsErrs = mean(abs(reshape(errs,[],size(us,5))));
282 ratioErrs = meanAbsErrs(2:end)./meanAbsErrs(1:end-1)

```

Plot solution in common patches First reshape arrays to suit 2D space surface plots, inserting nans to separate patches.

```

294 x = xs(:,:,1); y = ys(:,:,1); u=us;
295 x(end+1,:)=nan; y(end+1,:)=nan;
296 u(end+1,:,:)=nan; u(:,:,end+1,:)=nan;
297 u = reshape(permute(u,[1 3 2 4 5]),numel(x),numel(y),[]);

```

Plot the patch solution surfaces, with colour offset between surfaces (best if u -field has a range of one): blues are the full-domain solution, reds the coarsest patches.

```

305 figure(1), clf, colormap(jet)
306 for p=1:size(u,3)
307     mesh(x(:),y(:),u(:,:,p)',p+u(:,:,p)');
308     hold on;

```

```

309 end, hold off
310 view(60,55)
311 colorbar('Ticks',1:size(u,3) ...
312     , 'TickLabels', [num2str(nPs) ['x';'x';'x'] num2str(nPs)]);
313 xlabel('space x'), ylabel('space y'), zlabel('u(x,y)')
314 if0urCf2eps([mfilename 'us'])%optionally save

```

Plot error surfaces Plot the error surfaces, with colour offset between surfaces (best if u -field has a range of one): dark blue is the full-domain zero error, reds the coarsest patches.

```

326 err=u(:,:,:,1)-u;
327 maxAbsErr=max(abs(err(:)));
328 figure(2), clf, colormap(jet)
329 for p=1:size(u,3)
330     mesh(x(:),y(:),err(:,:,p)',p+err(:,:,p)'/maxAbsErr);
331     hold on;
332 end, hold off
333 view(60,55)
334 colorbar('Ticks',1:size(u,3) ...
335     , 'TickLabels', [num2str(nPs) ['x';'x';'x'] num2str(nPs)]);
336 xlabel('space x'), ylabel('space y')
337 zlabel('errors in u(x,y)')
338 if0urCf2eps(mfilename)%optionally save

```

3.18.1 twoscaleDiffForce2(): microscale discretisation inside patches of forced diffusion PDE

This function codes the lattice heterogeneous diffusion of the PDE inside the patches. For 6D input arrays u , x , and y , computes the time derivative at each point in the interior of a patch, output in ut .

```

357 function ut = twoscaleDiffForce2(t,u,patches)
358     dx = diff(patches.x(2:3)); % x space step
359     dy = diff(patches.y(2:3)); % y space step
360     i = 2:size(u,1)-1; % x interior points in a patch
361     j = 2:size(u,2)-1; % y interior points in a patch
362     ut = nan+u;           % preallocate output array

```

Set Dirichlet boundary value of zero around the square domain.

```

369 u( 1 ,:,:,:,:, 1 ,:) = 0; % left edge of left patches
370 u(end,:,:,:,end,:) = 0; % right edge of right patches
371 u(:, 1 ,:,:,:,:, 1 ) = 0; % bottom edge of bottom patches
372 u(:,end,:,:,:,end) = 0; % top edge of top patches

```

Compute the time derivatives via stored forcing and coefficients. Easier to code by conflating the last four dimensions into the one $,:$

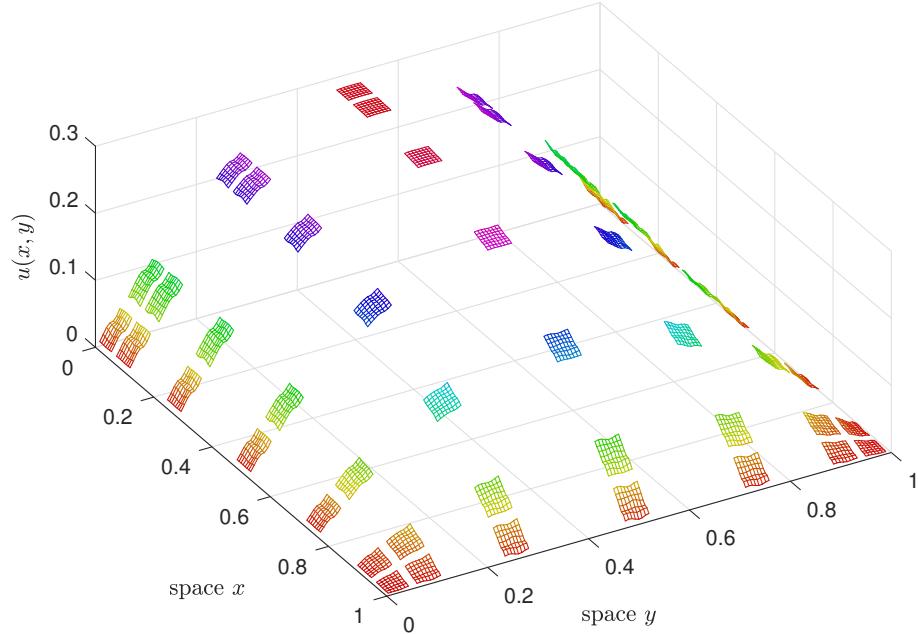
```

380 ut(i,j,:) ...
381 = 2*diff(u(:,j,:),2,1)/dx^2 +2*diff(u(i,:,:),2,2)/dy^2 ...
382     +2*patches.cs(i,j).*( u(i+1,j+1,:) - u(i-1,j+1,:) ...

```

```
383      -u(i+1,j-1,:) +u(i-1,j-1,:)) / (4*dx*dy) ...
384      +patches.fu(i,j,:);
385 end%function twoscaleDiffForce2
```

Figure 3.21: Equilibrium of the macroscale diffusion problem of Abdulle with boundary conditions of Dirichlet zero-value except for $x = 0$ which is Neumann (Section 3.19). Here the patches have a Chebyshev-like spatial distribution. The patch size is chosen large enough to see within.



3.19 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 3.21](#) shows solutions have some nice microscale wiggles reflecting the heterogeneity.

Clear, and initiate globals.

```
38 clear all
39 global patches
40 %global OurCf2eps, OurCf2eps=true %option to save plot
```

First establish the microscale heterogeneity has micro-period `mPeriod` on the spatial micro-grid lattice. Then `configPatches2` replicates the heterogeneity to fill each patch. (These diffusion coefficients should really recognise the half-grid-point shifts, but let’s not bother.)

```

53 mPeriod = 6
54 x = (0.5:mPeriod)'/mPeriod; y=x';
55 a = (2+1.8*sin(2*pi*x))./(2+1.8*sin(2*pi*y)) ...
56     +(2+
57 diffusivityRange = [min(a(:)) max(a(:))]
```

Set the periodicity ϵ , here big enough so we can see the patches, and other microscale parameters.

```

64 epsilon = 0.04
65 dx = epsilon/mPeriod
66 nPeriodsPatch = 1 % any integer
67 nSubP = nPeriodsPatch*mPeriod+2 % when edgy int
```

Patch configuration Choose either Dirichlet (default) or Neumann on the left boundary in coordination with micro-code in [Section 3.19.1](#)

```

78 Dom.bcOffset = zeros(2);
79 if 1, Dom.bcOffset(1)=0.5; end% left Neumann
```

Say use 7×7 patches in $(0, 1)^2$, fourth order interpolation, and either ‘equispace’ or ‘chebyshev’:

```

86 nPatch = 7
87 Dom.type='chebyshev';
88 configPatches2(@abdulleDiffForce2,[0 1],Dom ...
89 ,nPatch ,4 ,dx ,nSubP , 'EdgyInt',true , 'hetCoeffs',a );
```

Solve for steady state Set initial guess of zero, with NaN to indicate patch-edge values. Index i are the indices of patch-interior points, and the number of unknowns is then its length.

```

102 u0 = zeros(nSubP,nSubP,1,1,nPatch,nPatch);
103 u0([1 end],:,:) = nan; u0(:,[1 end],:) = nan;
104 patches.i = find(~isnan(u0));
105 nVariables = numel(patches.i)
```

Solve by iteration. Use `fsolve` for simplicity and robustness (and using `optimoptions` to omit trace information), via the generic patch system wrapper `theRes` ([Section 3.12](#)), and give magnitudes.

```

114 tic;
115 uSoln = fsolve(@theRes,u0(patches.i) ...
116                 ,optimoptions('fsolve','Display','off'));
117 solnTime = toc
118 normResidual = norm(theRes(uSoln))
119 normSoln = norm(uSoln)
```

Store the solution vector into the patches, and interpolate, but have not bothered to set boundary values so they stay NaN from the interpolation.

```

127 u0(patches.i) = uSoln;
128 u0 = patchEdgeInt2(u0);
```

Draw solution profile Separate patches with NaNs, then reshape arrays to suit 2D space surface plots.

```

139 figure(1), clf, colormap(0.8*hsv)
140 patches.x(end+1,:,:)=nan; u0(end+1,:,:)=nan;
141 patches.y(:,end+1,:)=nan; u0(:,end+1,:)=nan;
142 u = reshape(permute(squeeze(u0),[1 3 2 4]) ...
143     , [numel(patches.x) numel(patches.y)]);

```

Draw the patch solution surface, with boundary-values omitted as already NaN by not bothering to set them.

```

150 mesh(patches.x(:),patches.y(:,u')); view(60,55)
151 xlabel('space $x$'), ylabel('space $y$'), zlabel('$u(x,y)$')
152 ifOurCf2eps(mfilename) %optionally save plot

```

3.19.1 abdulleDiffForce2(): microscale discretisation inside patches of forced diffusion PDE

This function codes the lattice heterogeneous diffusion of the PDE inside the patches. For 6D input arrays u , x , and y , computes the time derivative at each point in the interior of a patch, output in ut .

```

171 function ut = abdulleDiffForce2(t,u,patches)
172     dx = diff(patches.x(2:3)); % x space step
173     dy = diff(patches.y(2:3)); % y space step
174     i = 2:size(u,1)-1; % x interior points in a patch
175     j = 2:size(u,2)-1; % y interior points in a patch
176     ut = nan+u;           % preallocate output array

```

Set Dirichlet boundary value of zero around the square domain, but also cater for zero Neumann condition on the left boundary.

```

184 u( 1 ,:,:, :, 1 ,:) = 0; % left edge of left patches
185 u(end,:,:,:,end,:) = 0; % right edge of right patches
186 u(:, 1 ,:,:, :, 1 ) = 0; % bottom edge of bottom patches
187 u(:,end,:,:,:,end) = 0; % top edge of top patches
188 if 1, u(1,:,:,:,1,:) = u(2,:,:,:,1,:); end% left Neumann

```

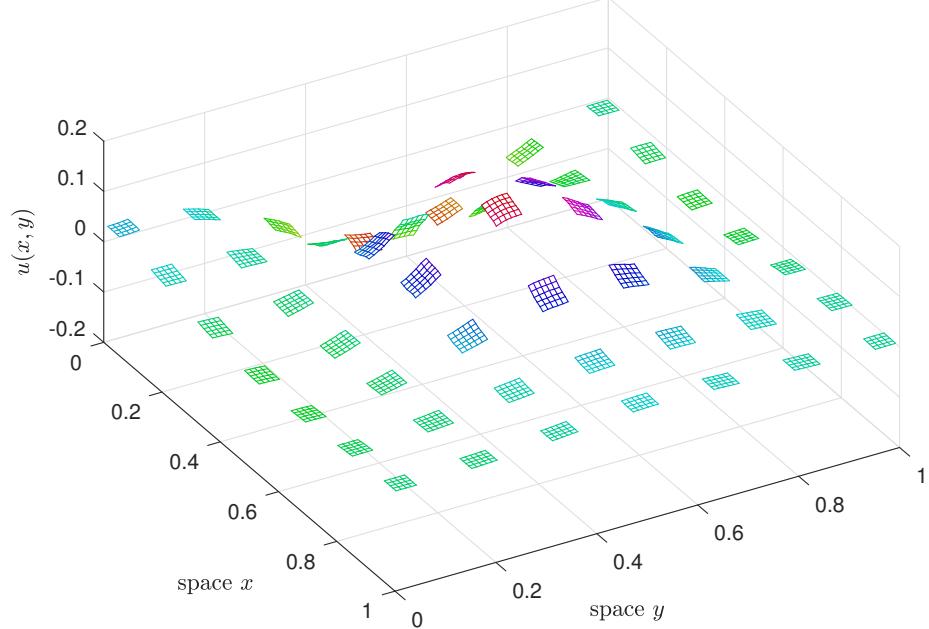
Compute the time derivatives via stored forcing and coefficients. Easier to code by conflating the last four dimensions into the one $,:$.

```

196 ut(i,j,:) = diff(patches.cs(:,j).*diff(u(:,j,:)))/dx^2 ...
197     + diff(patches.cs(i,:).*diff(u(i,:,:),1,2),1,2)/dy^2 ...
198     + 10;
199 end%function abdulleDiffForce2

```

Figure 3.22: Equilibrium of the macroscale diffusion problem of Bonizzoni et al. with Neumann boundary conditions of zero (Section 3.20). Here the patches have a equispaced spatial distribution. The microscale periodicity, and hence the patch size, is chosen large enough to see within.



3.20 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 3.22 plots one example. A physical interpretation of the solution field is confounded because the problem is pseudo-advection-diffusion due to the varying coefficients being outside the $\vec{\nabla}$ operator.

Clear, and initiate globals.

```
50 clear all
51 global patches
52 %global OurCf2eps, OurCf2eps=true %option to save plot
```

¹⁴ <http://arxiv.org/abs/2211.15221>

¹⁵ More interesting microscale structure arises here for μ_1 a factor of three smaller.

First establish the microscale heterogeneity has micro-period `mPeriod` on the spatial lattice. Then `configPatches2` replicates the heterogeneity to fill each patch.

```
63 mPeriod = 4
64 mu1 = 0.01*10.^rand(mPeriod)
65 mu2 = 2*pi*rand(mPeriod)
66 cs = cat(3,mu1,cos(mu2),sin(mu2));
67 meanDiffAdvec=squeeze(mean(mean(cs)))
```

Set the periodicity ϵ , here big enough so we can see the patches, and other microscale parameters.

```
74 epsilon = 0.04
75 dx = epsilon/mPeriod
76 nPeriodsPatch = 1 % any integer
77 nSubP = nPeriodsPatch*mPeriod+2 % for edgy int
```

Patch configuration Say use 7×7 patches in $(0, 1)^2$, fourth order interpolation, either ‘equispace’ or ‘chebyshev’, and the offset for Neumann boundary conditions:

```
89 nPatch = 7
90 Dom.type= 'equispace';
91 Dom.bcOffset = 0.5;
92 configPatches2(@randAdvecDiffForce2,[0 1],Dom ...
93 ,nPatch ,4 ,dx ,nSubP , 'EdgyInt',true , 'hetCoeffs',cs );
```

Compute the time-constant forcing, and store in struct `patches` for access by the microcode of [Section 3.20.1](#).

```
101 mu = [ 0.25+0.5*rand(1,2) 0.1+0.15*rand ]
102 patches.fu = exp(-((patches.x-mu(1)).^2 ...
103 +(patches.y-mu(2)).^2)/mu(3)^2);
```

Solve for steady state Set initial guess of zero, with `NaN` to indicate patch-edge values. Index `i` are the indices of patch-interior points, store in global `patches` for access by `theRes`, and the number of unknowns is then its number of elements.

```
118 u0 = zeros(nSubP,nSubP,1,1,nPatch,nPatch);
119 u0([1 end],:,:) = nan; u0(:,[1 end],:) = nan;
120 patches.i = find(~isnan(u0));
121 nVariables = numel(patches.i)
```

Solve by iteration. Use `fsolve` for simplicity and robustness (and using `optimoptions` to omit trace information), via the generic patch system wrapper `theRes` ([Section 3.12](#)).

```
130 tic;
131 uSoln = fsolve(@theRes,u0(patches.i) ...
132 ,optimoptions('fsolve','Display','off'));
133 solnTime = toc
```

```

134 normResidual = norm(theRes(uSoln))
135 normSoln = norm(uSoln)

```

Store the solution vector into the patches, and interpolate, but have not bothered to set boundary values so they stay NaN from the interpolation.

```

143 u0(patches.i) = uSoln;
144 u0 = patchEdgeInt2(u0);

```

Draw solution profile Separate patches with NaNs, then reshape arrays to suit 2D space surface plots.

```

155 figure(1), clf, colormap(0.8*hsv)
156 patches.x(end+1,:,:)=nan; u0(end+1,:,:)=nan;
157 patches.y(:,end+1,:)=nan; u0(:,end+1,:)=nan;
158 u = reshape(permute(squeeze(u0),[1 3 2 4]) ...
159     , [numel(patches.x) numel(patches.y)]);

```

Draw the patch solution surface, with boundary-values omitted as already NaN by not bothering to set them.

```

166 mesh(patches.x(:),patches.y(:),u'); view(60,55)
167 xlabel('space $x$'), ylabel('space $y$'), zlabel('$u(x,y)$')
168 ifOurCf2eps(mfilename) %optionally save plot

```

3.20.1 randAdvecDiffForce2(): microscale discretisation inside patches of forced diffusion PDE

This function codes the lattice heterogeneous diffusion of the PDE inside the patches. For 6D input arrays u , x , and y , computes the time derivative at each point in the interior of a patch, output in ut .

```

187 function ut = randAdvecDiffForce2(t,u,patches)
188     dx = diff(patches.x(2:3)); % x space step
189     dy = diff(patches.y(2:3)); % y space step
190     i = 2:size(u,1)-1; % x interior points in a patch
191     j = 2:size(u,2)-1; % y interior points in a patch
192     ut = nan+u;          % preallocate output array

```

Set Neumann boundary condition of zero derivative around the square domain: that is, the edge value equals the next-to-edge value.

```

200     u( 1 ,:,:, :, 1 ,:) = u( 2 ,:,:, :, 1 ,:); % left edge of left patches
201     u(end,:,:,:,end,:) = u(end-1,:,:,:,end,:); % right edge of right patches
202     u(:, 1 ,:,:, :, 1 ) = u(:, 2 ,:,:, :, 1 ); % bottom edge of bottom patches
203     u(:,end,:,:,:,end) = u(:,end-1,:,:,:,end); % top edge of top patches

```

Compute the time derivatives via stored forcing and coefficients. Easier to code by conflating the last four dimensions into the one $,:$.

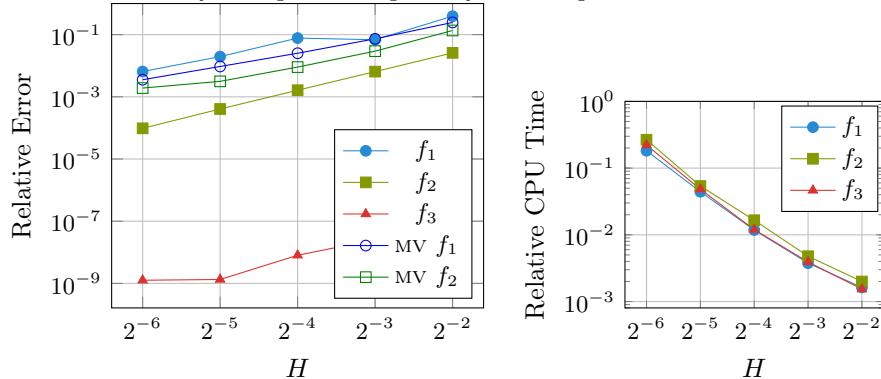
```

211     ut(i,j,:) ...
212     = patches.cs(i,j,1).*(diff(u(:,j,:),2,1)/dx^2 ...
213         +diff(u(:, :,1),2,2)/dy^2) ...
214         -patches.cs(i,j,2).*(u(i+1,j,:)-u(i-1,j,:))/(2*dx) ...

```

```
215      -patches.cs(i,j,3).*(u(i,j+1,:)-u(i,j-1,:))/(2*dy) ...
216      -u(i,j,:)+patches.fu(i,j,:);
217  end%function randAdvecDiffForce2
```

Figure 3.23: results for the computational homogenisation of a forced, non-autonomous, 2D wave (Section 3.21). (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.



3.21 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 ???. It favourably compares to the examples of Maier & Verfürth (2021).

Figure 3.23 summarises the results here. The left (larger) graph shows the error in the patch scheme decreasing with decreasing patch spacing H (increasing number of patches). Forcing f_1 and f_2 are as specified by §5.1 of Maier & Verfürth (2021), whereas f_3 here is f in their §5.2. For the case of forcing f_1 which is discontinuous in space (at $x = 0.4$), the errors are similar to that of Maier & Verfürth (2021)—compare the filled with unfilled circles. For the case of forcing f_2 which is continuous in the spatial domain, except for a second derivative discontinuity in its odd-periodic extension, the errors of the patch scheme are an order of magnitude better than that of Maier & Verfürth (2021)—compare the filled with unfilled squares. For the case of forcing f_3 which is smooth in the domain and in its odd-periodic extension, the patch scheme errors, roughly 10^{-8} , are at the tolerance of the time integration. Two caveats in a comparison with Maier & Verfürth (2021) are the slightly different norms used, and that they also address errors in the time integration, whereas here we use a standard adaptive integrator in order to focus purely on the spatial errors of the patch scheme.

Now let's code the simulation of the forced, non-autonomous, 2D wave. Maier & Verfürth (2021) have Dirichlet BCs of zero around the unit square, so replicate here by the odd periodic extension to the spatial domain $[-1, 1]^2$. In their §5.1, their microscale mesh step is $1/512 = 2^{-9}$. Coding that here results in a compute time of roughly 90 minutes, so here I provide a much coarser case that computes in only a few minutes: change as you please.

```

68 clear all
69 dx = 1/128 % 1/512=2^{-9} is the original, but takes 90 mins

```

The heterogeneity is of period four on the microscale lattice, so code a minimal patch size that covers one period.

```

77 epsilon = 4*dx
78 nPeriodsPatch = 1
79 mPeriod = round(epsilon/dx)
80 nSubP = mPeriod*nPeriodsPatch+2

```

Choose which of three forcing functions to use

```
86 fn=2
```

[Maier & Verfürth \(2021\)](#) use varying number of macroscale grid steps from 4 to 64 on $[0, 1]$ so here on $[-1, 1]$ we use double the number patches in each direction. Loop over the number of patches used, starting with the full domain simulation, and then progressively coarsening the macroscale grid of patches.

```

99 nPatch = 2/epsilon/nPeriodsPatch
100 for iPAt=0:9
101 if iPAt>0, nPatch=nPatch/2, end
102 if nPatch<8, break, end

```

Set the periodic heterogeneous coefficient, isotropic:

$$a_\epsilon(t, x) = [3 + \sin(2\pi x/\epsilon) + \sin(2\pi t)] \cdot [3 + \sin(2\pi y/\epsilon) + \sin(2\pi t)],$$

which being in product form with two time-dependencies we store as the two spatially varying factors—although to preserve odd symmetry we phase shift the heterogeneity from sines to cosines. It is a user’s choice whether to code such spatial dependencies here with `cHetr` or within the time derivative function itself. In this case, I choose to code microscale heterogeneous coefficients here via `cHetr`, and the macroscale variation of f_i in the time derivative function.

Here the period of the heterogeneity is only four microscale lattice points in each direction (which is pretty inaccurate on the microscale, but immaterial as we and [Maier & Verfürth \(2021\)](#) only compare to the coded system on the microscale lattice, not to the PDE). With the following careful choices we ensure all the hierarchy of patch schemes both maintain odd symmetry, and also compute on grid points that are common with the full domain.

```

130 ratio = (nSubP-2)*dx/(2/nPatch)
131 Xleft=(1-ratio)/nPatch;
132 xmid=Xleft+dx*(0:mPeriod-1)'; % half-points
133 xi = Xleft+dx*(-0.5:mPeriod-1)'; % grid-points
134 % two components for ax, the x-dirn interactions
135 cHetr(:,:,1) = (3+cos(2*pi*xmid/epsilon))+0*xi';
136 cHetr(:,:,2) = 0*xmid+(3+cos(2*pi*xi'/epsilon));
137 % two components for ay, the y-dirn interactions
138 cHetr(:,:,3) = (3+cos(2*pi*xi/epsilon))+0*xmid';
139 cHetr(:,:,4) = 0*xi+(3+cos(2*pi*xmid'/epsilon));

```

Configure patches using spectral interpolation. Quadratic interpolation did not seem significantly different for the case of discontinuous forcing f_1 .

```
148 configPatches2(@heteroWave2, [-1 1 -1 1], nan, nPatch ...
149     , 0, ratio, nSubP, 'EdgyInt', true, 'hetCoeffs', cHetr );
```

A check on the spatial geometry.

```
155 global patches
156 dxPat=diff(patches.x(1:2));
157 assert(abs(dx-dxPat)<1e-9, "dx mismatch")
```

Simulate Set the particular forcing function to use, and the zero initial conditions of a simulation.

```
167 patches.eff=fn;
168 clear uv0
169 uv0(:,:,1,1,:,:)= 0*patches.x+0*patches.y;
170 uv0(:,:,2,1,:,:)= 0*patches.x+0*patches.y;
```

Integrate using standard integrators. [Maier & Verfürth \(2021\)](#) use a scheme with fixed time-step of $\tau = 2^{-7} = 1/128$. Here `ode23` uses variable steps of about 0.0003, and takes 7 s for `nPatch=2*4` (whereas `ode15s` takes 149 s—even for the dissipating case), and takes 287 s for `nPatch=2*32` and roughly 4000 s for full domain `nPatch=2*128`.

```
182 disp('Now simulate over time')
183 tic
184 [ts,us] = ode23(@patchSys2, linspace(0,1,11), uv0(:));
185 if iPAt==0, odeTime0=toc
186 else relodeTime(iPat)=toc/odeTime0
187 end
```

Compute error compared to full domain simulation Get spatial coordinates of patch-interior points, and reshape to column vectors.

```
197 i = 2:nSubP-1;
198 x = squeeze(patches.x(i,:,:,:,:,:));
199 y = squeeze(patches.y(:,i,:,:,:,:));
200 x=x(:); y=y(:);
```

At the final time of $t = 1$, get the row vector of data, form into the 6D array via the interpolation to the edges, and reshape patch-interior points to 2D spatial array.

```
208 uv = squeeze(patchEdgeInt2(us(end,:)));
209 u = squeeze(uv(i,i,1,:,:));
210 u = reshape(permute(u,[1 3 2 4]),[numel(x) numel(y)]);
```

If this is the full domain simulation, then store as the reference solution.

```
217 if iPAt==0
218 x0=x; y0=y; u0=u;
```

```

219     rms0=sqrt(mean(u0(:).^2))
220 else
    Else compute the error compared to the full domain solution. First find
    the indices of the full domain that match the spatial locations of the patch
    scheme.

228 [i,k] = find(abs(x0-x')<1e-9);
229 assert(length(i)==length(x),'find error in index i')
230 [j,k] = find(abs(y0-y')<1e-9);
231 assert(length(j)==length(y),'find error in index j')

```

The RMS error over the surface is

```

237 errs=u-u0(i,j);
238 relrmserr(iPat)=sqrt(mean(errs(:).^2))/rms0
239 H(iPat)=2/nPatch
240 end%if iPat

```

End the loop over the various number of patches, and return. Further, here not executed, code in the file animates the solution over time, and computes spectrum of the system.

```

250 end%for iPat
251 figure(1), clf
252 loglog(H,relrmserr,'o:'), grid on
253 xlabel('H'), ylabel('relative error')
254 return

```

3.21.1 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 3.14](#)), computes the time derivative at each point in the interior of a patch, output in ut . The four 2D arrays of heterogeneous interaction coefficients, c_{ijk} , have previously been stored in `patches.cs` (3D).

Supply patch information as a third argument (required by parallel computation), or otherwise by a global variable.

```

26 function ut = heteroWave2(t,u,patches)
27 if nargin<3, global patches, end

```

Microscale space-steps, and interior point indices.

```

33 dx = diff(patches.x(2:3)); % x micro-scale step
34 dy = diff(patches.y(2:3)); % y micro-scale step
35 i = 2:size(u,1)-1; % x interior points in a patch
36 j = 2:size(u,2)-1; % y interior points in a patch
37 assert(max(abs(u(:)))<9999,"u-field exploding")

```

Form coefficients here—odd periodic extension. To avoid slight errors in periodicity (in full domain simulation), first adjust any coordinates crossing $x = \pm 1$ or $y = \pm 1$.

```
47 x=patches.x; y=patches.y;
48 l=find(abs(x)>1); x(l)=x(l)-sign(x(l))*2;
49 l=find(abs(y)>1); y(l)=y(l)-sign(y(l))*2;
```

Then set at this time three possible forcing functions, although only use one depending upon `patches.eff`. Forcing f_1 and f_2 are as specified by §5.1 of [Maier & Verfürth \(2021\)](#), whereas f_3 here is f in their §5.2.

```
59 f1 = ( (abs(x)>0.4)*(20*t+230*t^2) ...
60     +(abs(x)<0.4)*(100*t+2300*t^2) ).*sign(x).*sign(y);
61 f2 = 20*t*x.* (1-abs(x)).*y.* (1-abs(y)) ...
62     +230*t^2*(sign(y).*x.* (1-abs(x))+sign(x).*y.* (1-abs(y)));
63 f3 = (5*t+50*t^2)*sin(pi*x).*sin(pi*y);
```

Also set the heterogeneous interactions at this time.

```
69 ax = (patches.cs(:,:,1)+sin(2*pi*t)) ...
70     .* (patches.cs(:,:,2)+sin(2*pi*t));
71 ay = (patches.cs(:,:,3)+sin(2*pi*t)) ...
72     .* (patches.cs(:,:,4)+sin(2*pi*t));
```

Reserve storage (using `nan+u` appears quickest), and then assign time derivatives for interior patch values due to the heterogeneous interaction and forcing.

```
81 ut = nan+u; % preallocate output array
82 ut(i,j,1,:) = u(i,j,2,:);
83 ut(i,j,2,:) ...
84 = diff(ax(:,j).*diff(u(:,j,1,:),1),1)/dx^2 ...
85     +diff/ay(i,:).*diff(u(i,:,1,:),1,2),1,2)/dy^2 ...
86     +(patches.eff==1)*f1(i,j,:,:)
87     +(patches.eff==2)*f2(i,j,:,:)
88     +(patches.eff==3)*f3(i,j,:,:)
89     + 1e-4*(diff(u(:,j,2,:),2,1)/dx^2+diff(u(i,:,2,:),2,2)/dy^2);
90 end% function
```

In the last line above, the slight damping of 10^{-4} causes microscale modes to decay at rate e^{-28t} , with frequencies 2000–5000, whereas macroscale modes decay with rates roughly 0.0005–0.05 with frequencies 10–100. This slight damping term may correspond to the weak damping of the backward Euler scheme adopted by [Maier & Verfürth \(2021\)](#) for time integration.

3.22 configPatches3(): configures spatial patches in 3D

Section contents

3.22.1 If no arguments, then execute an example	110
3.22.2 heteroWave3(): heterogeneous Waves	112

Makes the struct `patches` for use by the patch/gap-tooth time derivative/step function `patchSys3()`, and possibly other patch functions. [Sections 3.22.1](#) and [3.25](#) list examples of its use.

```
20 function patches = configPatches3(fun,Xlim,Dom ...
21     ,nPatch,ordCC,dx,nSubP,varargin)
```

Input If invoked with no input arguments, then executes an example of simulating a heterogeneous wave PDE—see [Section 3.22.1](#) for an example code.

- `fun` is the name of the user function, `fun(t,u,patches)` or `fun(t,u)`, that computes time-derivatives (or time-steps) of quantities on the 3D micro-grid within all the 3D patches.
- `Xlim` array/vector giving the rectangular-cuboid macro-space domain of the computation: namely $[Xlim(1), Xlim(2)] \times [Xlim(3), Xlim(4)] \times [Xlim(5), Xlim(6)]$. If `Xlim` has two elements, then the domain is the cubic domain of the same interval in all three directions.
- `Dom` sets the type of macroscale conditions for the patches, and reflects the type of microscale boundary conditions of the problem. If `Dom` is `NaN` or `[]`, then the field `u` is triply macro-periodic in the 3D spatial domain, and resolved on equi-spaced patches. If `Dom` is a character string, then that specifies the `.type` of the following structure, with `.bcOffset` set to the default zero. Otherwise `Dom` is a structure with the following components.
 - `.type`, string, of either `'periodic'` (the default), `'equispace'`, `'chebyshev'`, `'usergiven'`. For all cases except `'periodic'`, users *must* code into `fun` the micro-grid boundary conditions that apply at the left/right/bottom/top/back/front faces of the left-most/rightmost/bottommost/topmost/backmost/frontmost patches, respectively.
 - `.bcOffset`, optional one, three or six element vector/array, in the cases of `'equispace'` or `'chebyshev'` the patches are placed so the left/right macroscale boundaries are aligned to the left/right faces of the corresponding extreme patches, but offset by `bcOffset` of the sub-patch micro-grid spacing. For example, use `bcOffset=0` when the micro-code applies Dirichlet boundary values on the extreme face micro-grid points, whereas use `bcOffset=0.5` when the microcode applies Neumann boundary conditions halfway

between the extreme face micro-grid points. Similarly for the top, bottom, back, and front faces.

If `.bcOffset` is a scalar, then apply the same offset to all boundaries. If three elements, then apply the first offset to both x -boundaries, the second offset to both y -boundaries, and the third offset to both z -boundaries. If six elements, then apply the first two offsets to the respective x -boundaries, the middle two offsets to the respective y -boundaries, and the last two offsets to the respective z -boundaries.

- `.X`, optional vector/array with `nPatch(1)` elements, in the case '`usergiven`' it specifies the x -locations of the centres of the patches—the user is responsible the locations makes sense.
- `.Y`, optional vector/array with `nPatch(2)` elements, in the case '`usergiven`' it specifies the y -locations of the centres of the patches—the user is responsible the locations makes sense.
- `.Z`, optional vector/array with `nPatch(3)` elements, in the case '`usergiven`' it specifies the z -locations of the centres of the patches—the user is responsible the locations makes sense.
- `nPatch` sets the number of equi-spaced spatial patches: if scalar, then use the same number of patches in all three directions, otherwise `nPatch(1:3)` gives the number (≥ 1) of patches in each direction.
- `ordCC` is the ‘order’ of interpolation for inter-patch coupling across empty space of the macroscale patch values to the face-values of the patches: currently must be 0, 2, 4, . . . ; where 0 gives spectral interpolation.
- `dx` (real—scalar or three elements) is usually the sub-patch micro-grid spacing in x , y and z . If scalar, then use the same `dx` in all three directions, otherwise `dx(1:3)` gives the spacing in each of the three directions.

However, if `Dom` is `NaN` (as for pre-2023), then `dx` actually is `ratio` (scalar or three elements), namely the ratio of (depending upon `EdgyInt`) either the half-width or full-width of a patch to the equi-spacing of the patch mid-points. So either $\text{ratio} = \frac{1}{2}$ 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 must be odd so that there is/are centre-patch micro-grid point/planes in each patch.
- ‘`nEdge`’ (not yet implemented), *optional*, default=1, for each patch, the number of face values set by interpolation at the face 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/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.
 - 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.¹⁶

```
217 if nargout==0, global patches, end
```

¹⁶ 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)` that computes the time derivatives (or steps) on the patchy lattice.
- `.ordCC` is the specified order of inter-patch coupling.
- `.periodic`: either true, for interpolation on the macro-periodic domain; or false, for general interpolation by divided differences over non-periodic domain or unevenly distributed patches.
- `.stag` is true for interpolation using only odd neighbouring patches as for staggered grids, and false for the usual case of all neighbour coupling—not yet implemented.
- `.Cwtsr` and `.Cwtsl` are the `ordCC × 3`-array of weights for the inter-patch interpolation onto the right/top/front and left/bottom/back faces (respectively) with patch:microscale ratio as specified or as derived from `dx`.
- `.x` (8D) is `nSubP(1) × 1 × 1 × 1 × 1 × nPatch(1) × 1 × 1` array of the regular spatial locations x_{iI} of the microscale grid points in every patch.
- `.y` (8D) is `1 × nSubP(2) × 1 × 1 × 1 × 1 × nPatch(2) × 1` array of the regular spatial locations y_{jJ} of the microscale grid points in every patch.
- `.z` (8D) is `1 × 1 × nSubP(3) × 1 × 1 × 1 × 1 × nPatch(3)` array of the regular spatial locations z_{kK} of the microscale grid points in every patch.
- `.ratio` 1×3 , only for macro-periodic conditions, are the size ratios of every patch.
- `.nEdge` is, for each patch, the number of face values set by interpolation at the face regions of each patch.
- `.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
 - 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.

3.22.1 If no arguments, then execute an example

```
305 if nargin==0
306 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 (" \leftrightarrow " denotes function recursion).

1. configPatches3
2. ode23 integrator \leftrightarrow patchSys3 \leftrightarrow 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.

```
324 mPeriod = [2 2 2];
325 cHetr = exp(0.9*randn([mPeriod 3]));
326 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.

```
338 global patches
339 patches = configPatches3(@heteroWave3, [-pi pi], 'periodic' ...
340 , 5, 0, 0.22, mPeriod+2, 'EdgyInt', true ...
341 , 'hetCoeffs', cHetr);
```

Set a wave initial state using auto-replication of the spatial grid, and as [Figure 3.24](#) shows. This wave propagates diagonally across space. Concatenate the two u, v -fields to be the two components of the fourth dimension.

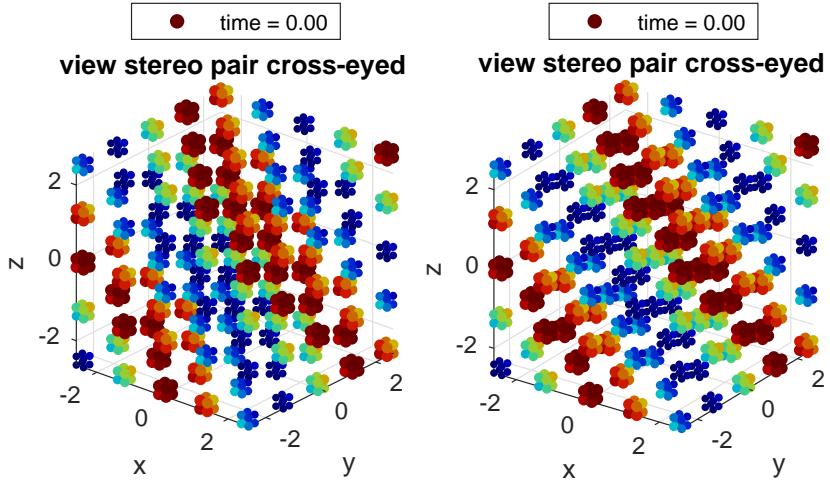
```
351 u0 = 0.5+0.5*sin(patches.x+patches.y+patches.z);
352 v0 = -0.5*cos(patches.x+patches.y+patches.z)*sqrt(3);
353 uv0 = cat(4,u0,v0);
```

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).

```
370 disp('Simulate heterogeneous wave u_tt=div[C*grad(u)]')
371 if ~exist('OCTAVE_VERSION', 'builtin')
372     [ts,us] = ode23(@patchSys3,linspace(0,6),uv0(:));
373 else %disp('octave version is very slow for me')
374     lsode_options('absolute tolerance',1e-4);
375     lsode_options('relative tolerance',1e-4);
376     [ts,us] = ode0cts(@patchSys3,[0 1 2],uv0(:));
377 end
```

Animate the computed simulation to end with [Figure 3.25](#). Use `patchEdgeInt3` to obtain patch-face values in order to most easily reconstruct the array data

Figure 3.24: initial field $u(x, y, z, t)$ at time $t = 0$ of the patch scheme applied to a heterogeneous wave PDE: [Figure 3.25](#) plots the computed field at time $t = 6$.



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.

```

391 figure(1), clf, colormap(0.8*jet)
392 xs = patches.x+0*patches.y+0*patches.z;
393 ys = patches.y+0*patches.x+0*patches.z;
394 zs = patches.z+0*patches.y+0*patches.x;
395 if 1, xs([1 end],:,:)=nan;
396     xs(:,[1 end],:,:)=nan;
397     xs(:,:,1 end,:)=nan;
398 end;%option
399 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.

```

407 pix = @(u) 15*abs(u)+7;
408 col = @(u) sign(u).*abs(u);

```

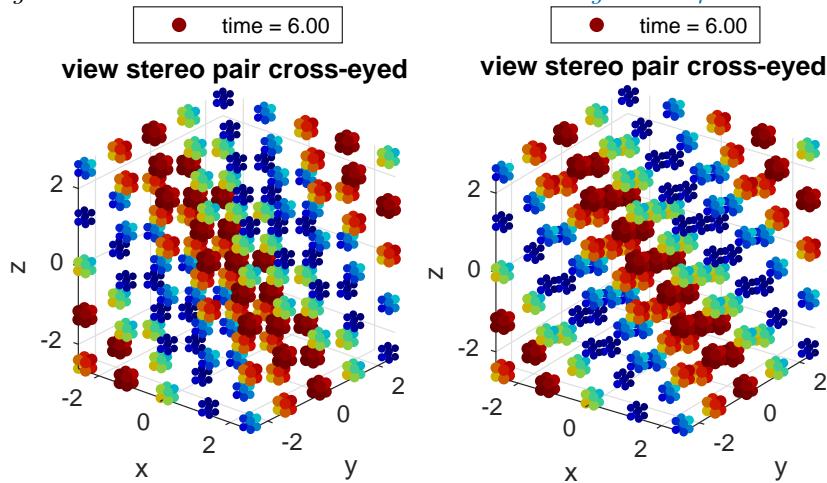
Loop to plot at each and every time step.

```

414 for i = 1:length(ts)
415     uv = patchEdgeInt3(us(i,:));
416     u = uv(:,:,1,:);
417     for p=1:2
418         subplot(1,2,p)
419         if (i==1)| exist('OCTAVE_VERSION','builtin')
420             scat(p) = scatter3(xs(j),ys(j),zs(j),'filled');
421             axis equal, caxis(col([0 1])), view(45-5*p,25)
422             xlabel('x'), ylabel('y'), zlabel('z')

```

Figure 3.25: 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 3.24.



```

423     title('view stereo pair cross-eyed')
424 end % in matlab just update values
425 set(scat(p), 'CData', col(u(j)) ...
426     , 'SizeData', pix((8+xs(j)-ys(j)+zs(j))/6+0*u(j)));
427 legend(['time = ' num2str(ts(i), '%4.2f')], 'Location', 'north')
428 end

```

Optionally save the initial condition to graphic file for Figure 3.15, and optionally save the last plot.

```

436 if i==1,
437     ifOurCf2eps([mfilename 'ic'])
438         disp('Type space character to animate simulation')
439         pause
440     else pause(0.05)
441     end
442 end% i-loop over all times
443 ifOurCf2eps([mfilename 'fin'])

```

Upon finishing execution of the example, exit this function.

```

458 return
459 end%if no arguments

```

3.22.2 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 3.23), computes the time derivative at each point in the interior of a patch, output in ut .

The three 3D array of heterogeneous coefficients, c_{ijk}^x , c_{ijk}^y and c_{ijk}^z , have previously been stored in `patches.cs` (4D).

Supply patch information as a third argument (required by parallel computation), or otherwise by a global variable.

```
26 function ut = heteroWave3(t,u,patches)
27 if nargin<3, global patches, end
```

Microscale space-steps, and interior point indices.

```
33 dx = diff(patches.x(2:3)); % x micro-scale step
34 dy = diff(patches.y(2:3)); % y micro-scale step
35 dz = diff(patches.z(2:3)); % z micro-scale step
36 i = 2:size(u,1)-1; % x interior points in a patch
37 j = 2:size(u,2)-1; % y interior points in a patch
38 k = 2:size(u,3)-1; % z interior points in a patch
```

Reserve storage and then assign interior patch values to the heterogeneous diffusion time derivatives. Using `nan+u` appears quicker than `nan(size(u),patches.codist)`

```
46 ut = nan+u; % preallocate output array
47 ut(i,j,k,1,:) = u(i,j,k,2,:);
48 ut(i,j,k,2,:) ...
49 =diff(patches.cs(:,j,k,1,:).*diff(u(:,j,k,1,:),1),1)/dx^2 ...
50 +diff(patches.cs(i,:,k,2,:).*diff(u(i,:,k,1,:),1,2),1,2)/dy^2 ...
51 +diff(patches.cs(i,j,:,:3,:).*diff(u(i,j,:,:1,:),1,3),1,3)/dz^2;
52 end% function
```

3.23 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. It assumes that the sub-patch structure is *smooth enough* so that the patch centre-values are sensible macroscale variables, and patch edge-values are determined by macroscale interpolation of the patch-centre or edge values. Nonetheless, microscale heterogeneous systems may be accurately simulated with this function via appropriate interpolation. Communicate patch-design variables (Section 3.22) either via the global struct `patches` or via an optional third argument (except that this last is required for parallel computing of `spmd`).

```
28 function dudt = patchSys3(t,u,patches)
29 if nargin<3, global patches, end
```

Input

- `u` is a vector/array of length $\text{prod}(\text{nSubP}) \cdot \text{nVars} \cdot \text{nEnsem} \cdot \text{prod}(\text{nPatch})$ where there are `nVars` · `nEnsem` field values at each of the points in the $\text{nSubP}(1) \times \text{nSubP}(2) \times \text{nSubP}(3) \times \text{nPatch}(1) \times \text{nPatch}(2) \times \text{nPatch}(3)$ spatial grid.
- `t` is the current time to be passed to the user's time derivative function.
- `patches` a struct set by `configPatches3()` with the following information used here.
 - `.fun` is the name of the user's function `fun(t,u,patches)` that computes the time derivatives on the patchy lattice. The array `u` has size $\text{nSubP}(1) \times \text{nSubP}(2) \times \text{nSubP}(3) \times \text{nVars} \times \text{nEsem} \times \text{nPatch}(1) \times \text{nPatch}(2) \times \text{nPatch}(3)$. Time derivatives must be computed into the same sized array, although herein the patch edge-values are overwritten by zeros.
 - `.x` is $\text{nSubP}(1) \times 1 \times 1 \times 1 \times \text{lnPatch}(1) \times 1 \times 1$ array of the spatial locations x_i of the microscale (i, j, k) -grid points in every patch. Currently it *must* be an equi-spaced lattice on both macro- and microscales.
 - `.y` is similarly $1 \times \text{nSubP}(2) \times 1 \times 1 \times 1 \times 1 \times \text{nPatch}(2) \times 1$ array of the spatial locations y_j of the microscale (i, j, k) -grid points in every patch. Currently it *must* be an equi-spaced lattice on both macro- and microscales.
 - `.z` is similarly $1 \times 1 \times \text{nSubP}(3) \times 1 \times 1 \times 1 \times \text{nPatch}(3)$ array of the spatial locations z_k of the microscale (i, j, k) -grid points in every patch. Currently it *must* be an equi-spaced lattice on both macro- and microscales.

Output

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

3.24 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.¹⁷

Communicate patch-design variables via a second argument (optional, except required for parallel computing of spmd), or otherwise via the global struct patches.

```
27 function u = patchEdgeInt3(u,patches)
28 if nargin<2, global patches, end
```

Input

- **u** is a vector/array of length $\text{prod}(\text{nSubP}) \cdot \text{nVars} \cdot \text{nEnsem} \cdot \text{prod}(\text{nPatch})$ where there are **nVars** · **nEnsem** field values at each of the points in the **nSubP1** · **nSubP2** · **nSubP3** · **nPatch1** · **nPatch2** · **nPatch3** multiscale spatial grid on the **nPatch1** · **nPatch2** · **nPatch3** array of patches.
- **patches** a struct set by configPatches3() which includes the following information.
 - **.x** is $\text{nSubP1} \times 1 \times 1 \times 1 \times 1 \times \text{nPatch1} \times 1 \times 1$ array of the spatial locations x_{iI} of the microscale grid points in every patch. Currently it *must* be an equi-spaced lattice on the microscale index i , but may be variable spaced in macroscale index I .
 - **.y** is similarly $1 \times \text{nSubP2} \times 1 \times 1 \times 1 \times 1 \times \text{nPatch2} \times 1$ array of the spatial locations y_{jJ} of the microscale grid points in every patch. Currently it *must* be an equi-spaced lattice on the microscale index j , but may be variable spaced in macroscale index J .
 - **.z** is similarly $1 \times 1 \times \text{nSubP3} \times 1 \times 1 \times 1 \times \text{nPatch3}$ array of the spatial locations z_{kK} of the microscale grid points in every patch. Currently it *must* be an equi-spaced lattice on the microscale index k , but may be variable spaced in macroscale index K .
 - **.ordCC** is order of interpolation, currently only $\{0, 2, 4, \dots\}$
 - **.periodic** indicates whether macroscale is periodic domain, or alternatively that the macroscale has left, right, top, bottom, front and back boundaries so interpolation is via divided differences.
 - **.stag** in $\{0, 1\}$ is one for staggered grid (alternating) interpolation. Currently must be zero.

¹⁷ 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).
- `.nEnsem` the number of realisations in the ensemble.
- `.parallel` whether serial or parallel.

Output

- `u` is 8D array, $n_{SubP1} \cdot n_{SubP2} \cdot n_{SubP3} \cdot n_{Vars} \cdot n_{Ensem} \cdot n_{Patch1} \cdot n_{Patch2} \cdot n_{Patch3}$, of the fields with face values set by interpolation.

3.25 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 ???. First set random heterogeneous diffusivities of random (small) period in each of the three directions. Crudely normalise by the harmonic mean so the decay time scale is roughly one.

```
29 mPeriod = randi([2 3],1,3)
30 cHetr = exp(0.3*randn([mPeriod 3]));
31 cHetr = cHetr*mean(1./cHetr(:))
```

Configure the patch scheme with some arbitrary choices of domain, patches, size ratios. Use spectral interpolation as we test other orders subsequently. In 3D we appear to get only real eigenvalues by using edgy interpolation. What happens for non-edgy interpolation is unknown.

```
42 nSubP=mPeriod+2;
43 nPatch=[5 5 5];
44 configPatches3(@heteroDiff3, [-pi pi], nan, nPatch ...
45 , 0, 0.3, nSubP, 'EdgyInt',true ...
46 , 'hetCoeffs',cHetr );
```

3.25.1 Simulate heterogeneous diffusion

Set initial conditions of a simulation as shown in [Figure 3.26](#).

```
56 global patches
57 u0 = exp(-patches.x.^2/4-patches.y.^2/2-patches.z.^2);
58 u0 = u0.*((1+0.3*rand(size(u0))));
```

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

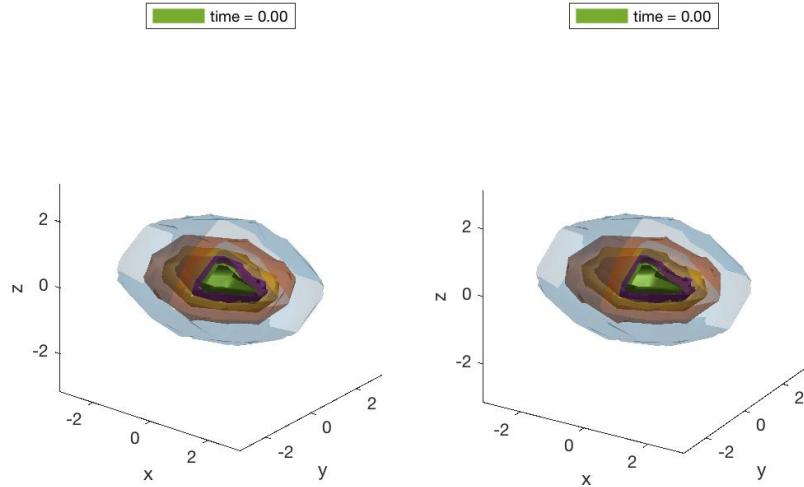
```
76 if ~exist('OCTAVE_VERSION','builtin')
77 [ts,us] = ode23(@patchSys3, 0.3*linspace(0,1,50).^2, u0(:));
78 else % octave version
79 [ts,us] = odeOcts(@patchSys3, 0.3*linspace(0,1).^2, u0(:));
80 end
```

Plot the solution as an animation over time.

```
88 figure(1), clf
89 rgb=get(gca,'defaultAxesColorOrder');
90 colormap(0.8*hsv)
```

Get spatial coordinates of patch interiors.

Figure 3.26: initial field $u(x, y, z, 0)$ of the patch scheme applied to a heterogeneous diffusion PDE. Plotted are the isosurfaces at field values $u = 0.1, 0.3, \dots, 0.9$, with the front quadrant omitted so you can see inside. Figure 3.27 plots the isosurfaces of the computed field at time $t = 0.3$.



```

96 x = reshape( patches.x([2:end-1],:,:, :) ,[],1);
97 y = reshape( patches.y(:,[2:end-1],:,:, :) ,[],1);
98 z = reshape( patches.z(:,:, [2:end-1],:) ,[],1);

```

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

```
105 for i = 1:length(ts)
```

Get the row vector of data, form into a 6D array, then omit patch faces, and reshape to suit the isosurface function. We do not use interpolation to get face values as the interpolation omits the corner edges and so breaks up the isosurfaces.

```

115 u = reshape( us(i,:), [nSubP nPatch]);
116 u = u([2:end-1],[2:end-1],[2:end-1],:,:,:);
117 u = reshape( permute(u,[1 4 2 5 3 6]) ...
118 , [numel(x) numel(y) numel(z)]);

```

Optionally cut-out the front corner so we can see inside.

```
124 u( (x>0) & (y'<0) & (shiftdim(z,-2)>0) ) = nan;
```

The `isosurface` function requires us to transpose x and y .

```
131 v = permute(u,[2 1 3]);
```

Draw cross-eyed stereo view of some isosurfaces.

```

137 clf;
138 for p=1:2
139 subplot(1,2,p)
140 for iso=5:-1:1
141 isov=(iso-0.5)/5;
142 hsurf(iso) = patch(isosurface(x,y,z,v, isov));
143 isonormals(x,y,z,v,hsurf(iso))
144 set(hsurf(iso) , 'FaceColor',rgb(iso,:)) ...
145 , 'EdgeColor','none' ...
146 , 'FaceAlpha',iso/5);
147 hold on
148 end
149 axis equal, view(45-7*p,25)
150 axis(pi*[-1 1 -1 1 -1 1])
151 xlabel('x'), ylabel('y'), zlabel('z')
152 legend(['time = ' num2str(ts(i),'%4.2f')], 'Location', 'north')
153 camlight, lighting gouraud
154 hold off
155 end% each p
156 if i==1 % pause for the viewer
157 makeJpeg=false;
158 if makeJpeg, print(['Figs/' mfilename 't0'], '-djpeg'), end
159 disp('Press any key to start animation of isosurfaces')
160 pause
161 else pause(0.05)
162 end
163
164
165
166
167
168 end%for over time
169 if makeJpeg, print(['Figs/' mfilename 'tFin'], '-djpeg'), end

```

Finish the animation loop, and optionally output the isosurfaces of the final field, [Figure 3.27](#).

3.25.2 Compute Jacobian and its spectrum

Let's explore the Jacobian dynamics for a range of orders of interpolation, all for the same random patch design and heterogeneity. Except here use a small ratio as we do not plot and then the scale separation is clearest.

```

195 ratio = 0.025*(1+rand(1,3))
196 nSubP=randi([3 5],1,3)
197 nPatch=[3 3 3]
198 nEnsem = prod(mPeriod) % or just set one

```

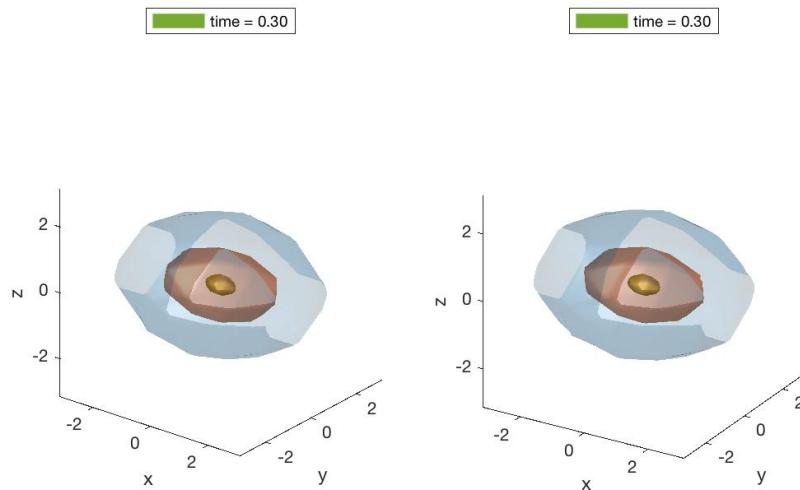
Find which elements of the 8D array are interior micro-grid points and hence correspond to dynamical variables.

```

205 u0 = zeros([nSubP,1,nEnsem,nPatch]);
206 u0([1 end],:,:,:)=nan;
207 u0(:,:,1,:)=nan;
208 u0(:,:,1,:)=nan;

```

Figure 3.27: final field $u(x, y, z, 0.3)$ of the patch scheme applied to a heterogeneous diffusion PDE. Plotted are the isosurfaces at field values $u = 0.1, 0.3, \dots, 0.9$, with the front quadrant omitted so you can see inside.



```

209 i = find(~isnan(u0));
210 sizeJacobian = length(i)
211 assert(sizeJacobian<4000 ...
212 , 'Jacobian is too big to quickly generate and analyse')

```

Store this many eigenvalues in array across different orders of interpolation.

```

219 nLeadEvals=prod(nPatch)+max(nPatch);
220 leadingEvals=[];

```

Evaluate eigenvalues for spectral as the base case for polynomial interpolation of order 2, 4,

```

228 maxords=6;
229 for ord=0:2:maxords
230     ord=ord

```

Configure with same heterogeneity.

```

236 configPatches3(@heteroDiff3, [-pi pi], nan, nPatch ...
237 , ord, ratio, nSubP, 'EdgyInt', true, 'nEnsem', nEnsem ...
238 , 'hetCoeffs', cHetr);

```

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

```

246 jac = nan(length(i));
247 for j = 1:length(i)

```

```

248      u = u0(:)+(i(j)==(1:numel(u0))');
249      tmp = patchSys3(0,u);
250      jac(:,j) = tmp(i);
251  end

```

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

```

258      notSymmetric=norm(jac-jac')
259  %    if notSymmetric>1e-7, spy(abs(jac-jac')>1e-7), end%??
260      assert(notSymmetric<1e-7,'failed symmetry')

```

Find all the eigenvalues (as `eigs` is unreliable), and put eigenvalues in a vector.

```

267      [evecs,evals] = eig((jac+jac')/2,'vector');
268      biggestImag=max(abs(imag(evals)));
269      if biggestImag>0, biggestImag=biggestImag, end

```

Sort eigenvalues on their real-part with most positive first, and most negative last. Store the leading eigenvalues in `egs`, and write out when computed all orders. The number of zero eigenvalues, `nZeroEv`, gives the number of decoupled systems in this patch configuration.

```

279      [~,k] = sort(-real(evals));
280      evals=evals(k); evecs=evecs(:,k);
281      if ord==0, nZeroEv=sum(abs(evals(:))<1e-5), end
282      if ord==0, evec0=evecs(:,1:nZeroEv*nLeadEvals);
283      else % find evec closest to that of each leading spectral
284          [~,k]=max(abs(evecs'*evec0));
285          evals=evals(k); % re-sort in corresponding order
286      end
287      leadingEvals=[leadingEvals evals(nZeroEv*(1:nLeadEvals))];
288  end
289  disp('    spectral    quadratic    quartic    sixth-order ...')
290  leadingEvals=leadingEvals

```

3.25.3 `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 3.23), computes the time derivative (3.1) at each point in the interior of a patch, output in `ut`. The three 3D array of diffusivities, c_{ijk}^x , c_{ijk}^y and c_{ijk}^z , have previously been stored in `patches.cs` (4+D).

Supply patch information as a third argument (required by parallel computation), or otherwise by a global variable.

```

23  function ut = heteroDiff3(t,u,patches)
24      if nargin<3, global patches, end
25
26      Microscale space-steps. Q: is using i,j,k slower than 2:end-1??
27
28      dx = diff(patches.x(2:3)); % x micro-scale step
29      dy = diff(patches.y(2:3)); % y micro-scale step

```

```

33      dz = diff(patches.z(2:3)); % z micro-scale step
34      i = 2:size(u,1)-1; % x interior points in a patch
35      j = 2:size(u,2)-1; % y interior points in a patch
36      k = 2:size(u,3)-1; % z interior points in a patch

```

Reserve storage and then assign interior patch values to the heterogeneous diffusion time derivatives. Using `nan+u` appears quicker than `nan(size(u),patches.codist)`

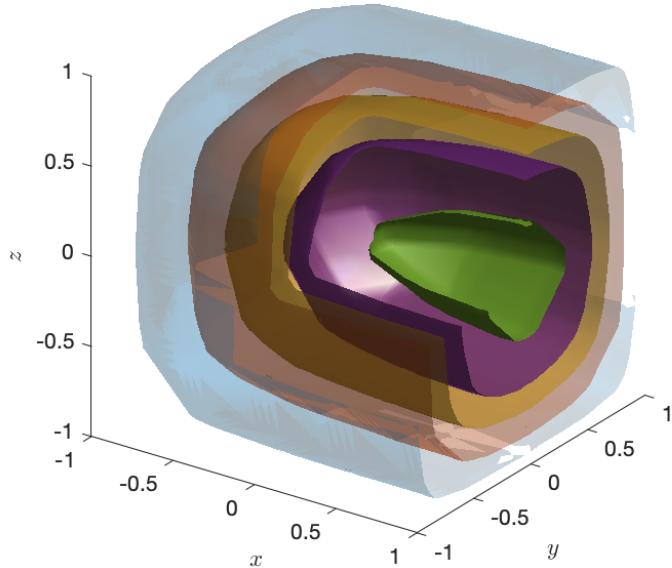
```

44      ut = nan+u; % reserve storage
45      ut(i,j,k,:,:,:,:, :) ...
46      = diff(patches.cs(:,j,k,1,:).*diff(u(:,j,k,:,:,:,:,:),1),1)/dx^2 ...
47      +diff(patches.cs(i,:,k,2,:).*diff(u(i,:,k,:,:,:,:,:),1,2),1,2)/dy^2 ...
48      +diff(patches.cs(i,j,:,3,:).*diff(u(i,j,:,:,:,:,:),1,3),1,3)/dz^2;
49  end% function

```

Fin.

Figure 3.28: 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 3.26). The small patches are equispaced in space.



3.26 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 3.28 shows five isosurfaces of the 3D solution field.

Clear variables, and establish globals.

```

33 clear all
34 global patches
35 %global OurCf2eps, OurCf2eps=true %option to save plots

```

Set random heterogeneous diffusivities of random (small) period in each of the three directions. Crudely normalise by the harmonic mean so the decay time scale is roughly one.

```

46 mPeriod = randi([2 3],1,3)
47 cDiff = exp(0.3*randn([mPeriod 3]));
48 cDiff = cDiff*mean(1./cDiff(:))

```

Configure the patch scheme with some arbitrary choices of cubic domain, patches, and micro-grid spacing 0.05. Use high order interpolation as few patches in each direction. Configure for Dirichlet boundaries except for Neumann on the right x -face.

```

59 nSubP = mPeriod+2;
60 nPatch = 5;
61 Dom.type = 'equispace';
62 Dom.bcOffset = zeros(2,3); Dom.bcOffset(2) = 0.5;
63 configPatches3(@microDiffBdry3, [-1 1], Dom ...
64 , nPatch, 0, 0.05, nSubP, 'EdgyInt',true ...
65 , 'hetCoeffs',cDiff );

```

Set forcing, and store in global patches for access by the microcode

```

73 patches.fu = 10*exp(-patches.x.^2-patches.y.^2-patches.z.^2);
74 patches.fu = patches.fu.* (1+rand(size(patches.fu)));

```

Solve for steady state Set initial guess of zero, with NaN to indicate patch-edge values. Index i are the indices of patch-interior points, store in global patches for access by theRes, and the number of unknowns is then its number of elements.

```

87 u0 = zeros([nSubP,1,1,nPatch,nPatch]);
88 u0([1 end],:,:, :) = nan;
89 u0(:,[1 end],:,:) = nan;
90 u0(:,:, [1 end],:) = nan;
91 patches.i = find(~isnan(u0));
92 nVariables = numel(patches.i)

```

Solve by iteration. Use fsolve for simplicity and robustness (optionally optimoptions to omit trace information), via the generic patch system wrapper theRes (Section 3.12).

```

101 disp('Solving system, takes 10--40 secs'),tic
102 uSoln = fsolve(@theRes,u0(patches.i) ...
103 ,optimoptions('fsolve','Display','off'));
104 solveTime = toc
105 normResidual = norm(theRes(uSoln))
106 normSoln = norm(uSoln)

```

Store the solution into the patches, and give magnitudes.

```

112 u0(patches.i) = uSoln;
113 u0 = patchEdgeInt3(u0);

```

Plot isosurfaces of the solution

```

122 figure(1), clf
123 rgb=get(gca,'defaultAxesColorOrder');

```

Reshape spatial coordinates of patches.

```

129 x = patches.x(:); y = patches.y(:); z = patches.z(:);

```

Draw isosurfaces. Get the solution with interpolated faces, form into a 6D array, and reshape and transpose x and y to suit the isosurface function.

```

137 u = reshape( permute(squeeze(u0),[2 5 1 4 3 6]) ...
138     , [numel(y) numel(x) numel(z)]);
139 maxu=max(u(:)), minu=min(u(:))

    Optionally cut-out the front corner so we can see inside.

145 u( (x'>0) & (y<0) & (shiftdim(z,-2)>0) ) = nan;

    Draw some isosurfaces.

151 clf;
152 for iso=5:-1:1
153     isov=(iso-0.5)/5*(maxu-minu)+minu;
154     hsurf(iso) = patch(isosurface(x,y,z,u,isov));
155     isonormals(x,y,z,u,hsurf(iso))
156     set(hsurf(iso) , 'FaceColor',rgb(iso,:)
157         , 'EdgeColor','none' , 'FaceAlpha',iso/5);
158     hold on
159 end
160 hold off
161 axis equal, axis([-1 1 -1 1 -1 1]), view(35,25)
162 xlabel('$x$'), ylabel('$y$'), zlabel('$z$')
163 camlight, lighting gouraud
164 if OurCf2eps(mfilename) %optionally save plot
165 if exist('OurCf2eps') && OurCf2eps, print('-dpng',[ 'Figs/' mfilename]), end

```

3.26.1 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 3.23](#)), computes the time derivative at each point in the interior of a patch, output in ut . The three 3D array of diffusivities, c_{ijk}^x , c_{ijk}^y and c_{ijk}^z , have previously been stored in `patches.cs` (4D).

Supply patch information as a third argument (required by parallel computation), or otherwise by a global variable.

```

191 function ut = microDiffBdry3(t,u,patches)
192 if nargin<3, global patches, end

    Microscale space-steps.

198 dx = diff(patches.x(2:3)); % x micro-scale step
199 dy = diff(patches.y(2:3)); % y micro-scale step
200 dz = diff(patches.z(2:3)); % z micro-scale step
201 i = 2:size(u,1)-1; % x interior points in a patch
202 j = 2:size(u,2)-1; % y interior points in a patch
203 k = 2:size(u,3)-1; % z interior points in a patch

```

Code microscale boundary conditions of say Neumann on right, and Dirichlet on left, top, bottom, front, and back (viewed along the z -axis).

```

211    u( 1 ,:,:, :, :, 1 ,:,:) = 0; %left face of leftmost patch
212    u(end,:,:, :, :,end,:,:) = u(end-1,:,:, :, :,end,:,:); %right face of rightmost
213    u(:, 1 ,:,:, :, :, 1 ,:) = 0; %bottom face of bottommost
214    u(:,end,:,:, :, :,end,:,:) = 0; %top face of topmost
215    u(:, :, 1 ,:,:, :, :, 1 ) = 0; %front face of frontmost
216    u(:, :,end,:,:, :, :,end) = 0; %back face of backmost

```

Reserve storage and then assign interior patch values to the heterogeneous diffusion time derivatives. Using `nan+u` appears quicker than `nan(size(u),patches.codist)`

```

224    ut = nan+u; % reserve storage
225    ut(i,j,k,:)
226    = diff(patches.cs(:,j,k,1).*diff(u(:,j,k,:),1,1),1,1)/dx^2 ...
227      +diff(patches.cs(i,:,k,2).*diff(u(i,:,k,:),1,2),1,2)/dy^2 ...
228      +diff(patches.cs(i,j,:,:3).*diff(u(i,j,:,:3),1,3),1,3)/dz^2 ...
229      +patches.fu(i,j,k);
230  end% function

```

4 Matlab parallel computation of the patch scheme

Chapter contents

4.1	<code>chanDispSpmd</code> : simulation of a 1D shear dispersion via simulation on small patches across a channel	130
4.1.1	Simulate heterogeneous advection-diffusion	132
4.1.2	Plot the solution	134
4.1.3	<code>microBurst</code> function for Projective Integration	135
4.1.4	<code>chanDispMicro()</code> : heterogeneous 2D advection-diffusion in a long thin channel	136
4.2	<code>rotFilmSpmd</code> : simulation of a 2D shallow water flow on a rotating heterogeneous substrate	138
4.2.1	Simulate heterogeneous advection-diffusion	139
4.2.2	Plot the solution	142
4.2.3	<code>microBurst</code> function for Projective Integration	143
4.2.4	<code>rotFilmMicro()</code> : 2D shallow water flow on a rotating heterogeneous substrate	144
4.3	<code>homoDiff31spmd</code> : computational homogenisation of a 1D dispersion via parallel simulation on small 3D patches of heterogeneous diffusion	146
4.3.1	Simulate heterogeneous diffusion	147
4.3.2	Plot the solution	149
4.3.3	<code>microBurst</code> function for Projective Integration	150
4.4	<code>RK2mesoPatch()</code>	152

For large-scale simulations, we here assume you have a compute cluster with many independent computer processors linked by a high-speed network. The functions we provide in our toolbox aim to distribute computations in parallel across the cluster. MATLAB's *Parallel Computing Toolbox* empowers a reasonably straightforward way to implement this parallelisation.¹ The reason is that the patch scheme (Chapter 3) has a clear domain decomposition of assigning relatively few patches to each processor.

¹ This parallelisation is not written for, nor tested for, Octave.

The examples listed herein are all *Proof of Principle*: as coded they are all small enough that non-parallel execution is here much quicker than the parallel execution. One needs significantly larger and/or more detailed problems than these examples before parallel execution is effective.

As in all parallel cluster computing, interprocessor communication time all too often dominates. It is important to reduce communication as much as possible compared to computation. Consequently, parallel computing is only effective when there is a very large amount of microscale computation done on each processor per communication—all of the examples listed herein are quite small and so the parallel computation of these is much slower than serial computation. We guesstimate that the microscale code may need, per time-step, of the order of many millions of operations per processor in order for the parallelisation to be useful.

To help minimise communication in time-dependent problems we have drafted a special integrator `RK2mesoPatch`, [Section 4.4](#), that communicates between patches only on a meso-time ([Bunder et al. 2016](#)).

4.1 chanDispSpmd: simulation of a 1D shear dispersion via simulation on small patches across a channel

Section contents

4.1.1	Simulate heterogeneous advection-diffusion	132
4.1.2	Plot the solution	134
4.1.3	microBurst function for Projective Integration	135
4.1.4	chanDispMicro(): heterogeneous 2D advection-diffusion in a long thin channel	136

Simulate 1D shear dispersion along long thin channel, dispersion that is emergent from micro-scale dynamics in 2D space. Use 1D patches as a Proof of Principle example of parallel computing with `spmd`. In this shear dispersion, although the micro-scale diffusivities are one-ish, the shear causes an effective longitudinal ‘diffusivity’ of the order of Pe^2 —which is typically much larger than the micro-scale diffusivity (Taylor 1953, e.g.).

The spatial domain is the channel (large) L -periodic in x and $|y| < 1$. Seek to predict a concentration field $c(x, y, t)$ satisfying the linear advection-diffusion PDE

$$\frac{\partial c}{\partial t} = -\text{Pe} u(y) \frac{\partial c}{\partial x} + \frac{\partial}{\partial x} \left[\kappa_x(y) \frac{\partial c}{\partial x} \right] + \frac{\partial}{\partial y} \left[\kappa_y(y) \frac{\partial c}{\partial y} \right]. \quad (4.1)$$

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 (4.1) is then

$$\begin{aligned} \frac{\partial c_{ij}}{\partial t} &= -\text{Pe} u(y_j) \frac{c_{i+1,j} - c_{i-1,j}}{2\delta x} + \frac{d_{i,j+1/2} - d_{i,j-1/2}}{\delta y} + \frac{D_{i+1/2,j} - D_{i-1/2,j}}{\delta x}, \\ d_{ij} &:= \kappa_y(y_j) \frac{c_{i,j+1/2} - c_{i,j-1/2}}{\delta y}, \quad D_{ij} := \kappa_x(y_j) \frac{c_{i+1/2,j} - c_{i-1/2,j}}{\delta x}. \end{aligned} \quad (4.2)$$

These are coded in Section 4.1.4 for the computation.

Choose one of four cases:

- `theCase=1` is corresponding code without parallelisation (in this toy problem it is much the quickest because there is no expensive interprocessor communication);
- `theCase=2` illustrates that `RK2mesoPatch` invokes `spmd` computation if parallel has been configured.
- `theCase=3` shows how users explicitly invoke `spmd`-blocks around the time integration.

- `theCase=4` invokes projective integration for long-time simulation via short bursts of the micro-computation, bursts done within `spmd`-blocks for parallel computing.

First, clear all to remove any existing globals, old composites, etc—although a parallel pool persists. Then choose the case.

```
75  clear all
76  theCase = 1
```

The micro-scale PDE is evaluated at positions y_j across the channel, $|y| < 1$. The even indexed points are the collocation points for the PDE, whereas the odd indexed points are the half-grid points for specification of y -diffusivities.

```
86  ny = 7
87  y = linspace(-1,1,2*ny+1);
88  yj = y(2:2:end);
```

Set micro-scale advection (array 1) and diffusivity (array 2) with (roughly) parabolic shape (Watt & Roberts 1995, MacKenzie & Roberts 2003, e.g.). Here modify the parabola by a heterogeneous log-normal factor with specified period along the channel: modify the strength of the heterogeneity by the coefficient of `randn` from zero to perhaps one: coefficient 0.3 appears a good moderate value. Remember that `configPatches1` reshapes `cHetr` to 2D.

```
101 mPeriod = 4
102 cHetr = shiftdim([3/2 1], -1).* (1-y.^2) ...
103 . *exp(0.3*randn([mPeriod 2*ny+1 2]));
```

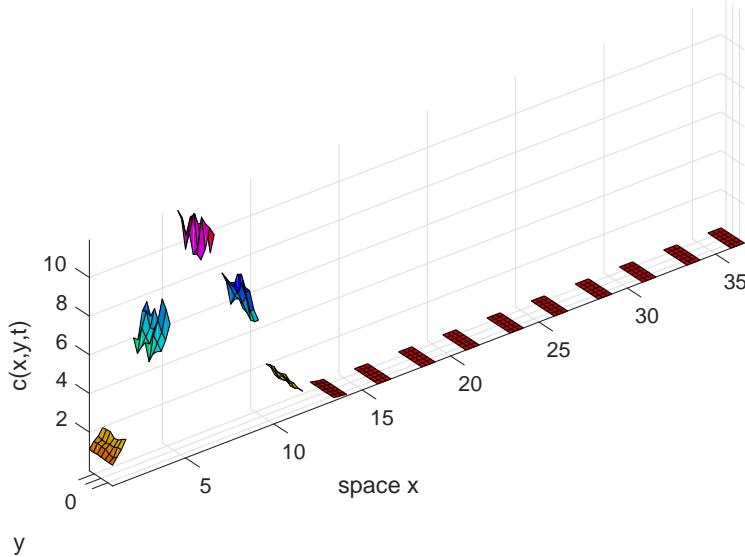
Configure the patch scheme with some arbitrary choices of domain, patches, size ratios. Choose some random order of interpolation to see the alternatives. Set `patches` information to be global so the info can be used for Cases 1–2 without being explicitly passed as arguments. Choose the parallel option if not Case 1, which invokes `spmd`-block internally, so that field variables become *distributed* across cpus.

```
118 if theCase<=2, global patches, end
119 nPatch=15
120 nSubP=2+mPeriod
121 ratio=0.2+0.2*(theCase<4)
122 Len=nPatch/ratio
123 ordCC=2*randi([0 3])
124 disp('**** Setting configPatches1')
125 patches = configPatches1(@chanDispMicro, [0 Len], nan ...
126 , nPatch, ordCC, ratio, nSubP, 'EdgyInt',true ...
127 , 'hetCoeffs',cHetr , 'parallel',(theCase>1) );
```

When using parallel then additional parameters to `patches` should be set within a `spmd` block (because `patches` is a co-distributed structure).

```
135 Peclet = 10
136 if theCase==1, patches.Pe = Peclet;
137 else      spmd, patches.Pe = Peclet; end
138 end
```

Figure 4.1: initial field $u(x, y, 0)$ of the patch scheme applied to a heterogeneous advection-diffusion PDE. Figure 4.2 plots the roughly smooth field values at time $t = 4$. In this example the patches are relatively large, ratio 0.4, for visibility.



4.1.1 Simulate heterogeneous advection-diffusion

Set initial conditions of a simulation as shown in Figure 4.1.

```
149 disp('**** Set initial condition and test dc0dt =')
150 if theCase==1
```

Without parallel processing, invoke the usual operations.

```
156     c0 = 10*exp(-(ratio*patches.x-2.5).^2/2) +0*yj;
157     c0 = c0.*(1+0.2*rand(size(c0)));
158     dc0dt = patchSys1(0,c0);
```

With parallel, we must use an `spmd`-block for computations: there is no difference in cases 2–4 here. Also, we must sometimes use `patches.codist` to explicitly code how to distribute new arrays over the cpus. Now `patchSys1` does not invoke `spmd` so higher level code must, as here. Even if `patches` is global, inside `spmd`-block we *must* pass it explicitly as a parameter to `patchSys1`.

```
171 else, spmd
172     c0 = 10*exp(-(ratio*patches.x-2.5).^2/2) +0*yj;
173     c0 = c0.*(1+0.2*rand(size(c0),patches.codist));
174     dc0dt = patchSys1(0,c0,patches)
175     end%spmd
176 end%if theCase
```

Integrate in time, either via the automatic `ode23` or via `RK2mesoPatch` which reduces communication between patches. By default, `RK2mesoPatch` does ten micro-steps for each specified meso-step in `ts`. For stability: with noise up

to 0.3, need micro-steps less than 0.005; with noise 1, need micro-steps less than 0.0015.

```
198 warning('Integrating system in time, wait patiently')
199 ts=4*linspace(0,1);
```

Go to the selected case.

```
205 switch theCase
```

1. For non-parallel, we could use `RK2mesoPatch` as indicated below, but instead choose to use standard `ode23` as here `patchSys1` accesses patch information via global `patches`. For post-processing, reshape each and every row of the computed solution to the correct array size—namely that of the initial condition.

```
217 case 1
218 % [cs,uerrs] = RK2mesoPatch(ts,c0);
219 [ts,cs] = ode23(@patchSys1,ts,c0(:));
220 cs=reshape(cs,[length(ts) size(c0)]);
```

2. In the second case, `RK2mesoPatch` detects a parallel patch code has been requested, but has only one cpu worker, so it auto-initiates an `spmd`-block for the integration. Both this and the next case return *composite* results, so just keep one version of the results.

```
232 case 2
233 cs = RK2mesoPatch(ts,c0);
234 cs = cs{1};
```

3. In this third case, a user could merge this explicit `spmd`-block with the previous one that sets the initial conditions.

```
243 case 3,spmd
244 cs = RK2mesoPatch(ts,c0,[],patches);
245 end%spmd
246 cs = cs{1};
```

4. In this fourth case, use Projective Integration (PI) over long times (`PIRK4` also works). Currently the PI is done serially, with parallel `spmd`-blocks only invoked inside function `aBurst()` ([Section 4.3.3](#)) 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 4.1.3](#)) in order to provide shaped initial states, and to provide the patch information.

```
264 case 4
265 microBurst = @(tb0,xb0,bT) ...
266     aBurst(tb0 ,reshape(xb0,size(c0)) ,patches);
267 ts = 0:0.7:5
268 cs = PIRK2(microBurst,ts,gather(c0(:)));
269 cs = reshape(cs,[length(ts) size(c0)]);
```

End the four cases.

```
276 end%switch theCase
```

4.1.2 Plot the solution

Optionally set to save some plots to file.

```
287 if 0, global OurCf2eps, OurCf2eps=true, end
```

Animate the computed solution field over time

```
293 figure(1), clf, colormap(0.8* hsv)
```

First get the x -coordinates and omit the patch-edge values from the plot (because they are not here interpolated).

```
301 if theCase==1, x = patches.x;
302 else, spmd
303     x = gather( patches.x );
304 end%spmd
305     x = x{1};
306 end
307 x([1 end],:,:, :) = nan;
```

For every time step draw the concentration values as a set of surfaces on 2D patches, with a short pause to display animation.

```
315 nTimes = length(ts)
316 for l = 1:nTimes
```

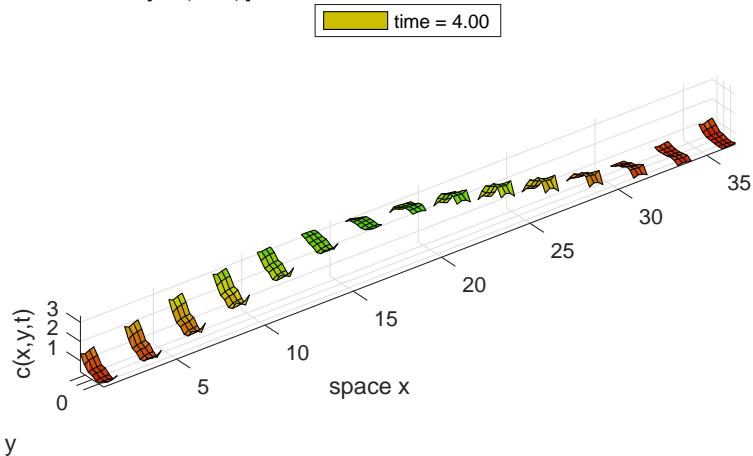
At each time, squeeze sub-patch data into a 3D array, permute to get all the x -variation in the first two dimensions, and reshape into x -variation for each and every (y).

```
325 c = reshape( permute( squeeze( ...
326     cs(l,:,:,:, :) ) , [1 3 2] ) ,numel(x) ,ny);
```

Draw surface of each patch, to show both micro-scale and macro-scale variation in space.

```
333 if l==1
334     hp = surf(x(:,yj,c'));
335     axis([0 Len -1 1 0 max(c(:))])
336     axis equal
337     xlabel('space x'), ylabel('y'); zlabel('c(x,y,t)')
338     ifOurCf2eps([mfilename 't0'])
339     legend(['time = ' num2str(ts(l),'%4.2f')] ...
340         , 'Location','north')
341     disp('**** pausing, press blank to animate')
342     pause
343 else
344     hp.ZData = c';
345     legend(['time = ' num2str(ts(l),'%4.2f')])
```

Figure 4.2: final field $c(x, y, 4)$ of the patch scheme applied to a heterogeneous advection-diffusion PDE (4.1) with heterogeneous factor log-normal, here distributed $\exp[\mathcal{N}(0, 1)]$.



```
346     pause(0.1)
347 end
```

Finish the animation loop, and optionally save the final plot to file, [Figure 4.2](#).

```
363 end%for over time
364 ifOurCf2eps([mfilename 'tFin'])
```

Macro-scale view Plot a macro-scale mesh of the predictions: at each of a selection of times, for every patch, plot the patch-mean value at the mean- x .

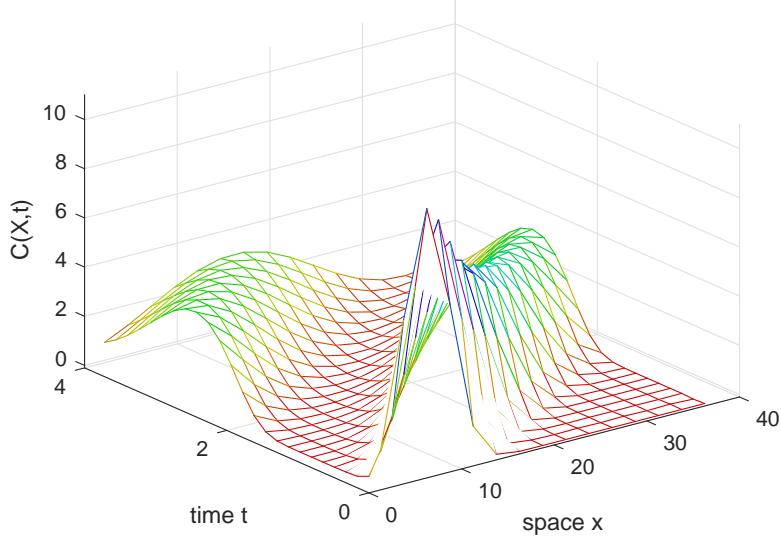
```
374 figure(2), clf, colormap(0.8*hsv)
375 X = squeeze(mean(x(2:end-1,:,:,:)));
376 C = squeeze(mean(mean(cs(:,2:end-1,:,:,:),2),3));
377 j = 1:ceil(nTimes/30):nTimes;
378 mesh(X,ts(j),C(j,:));
379 xlabel('space x'), ylabel('time t'), zlabel('C(X,t)')
380 zlim([-0.1 11])
381 ifOurCf2eps([mfilename 'Macro'])
```

4.1.3 microBurst function for Projective Integration

Projective Integration stability appears to require bursts longer than 0.2. Each burst is done in parallel processing. Here use RK2mesoPatch to take meso-steps, each with default ten micro-steps so the micro-scale step is 0.0033. With macro-step 0.5, these parameters usually give stable projective integration.

```
404 function [tbs,xbs] = aBurst(tb0,xb0,patches)
405     normx=max(abs(xb0(:)));
406     disp(['* aBurst t=' num2str(tb0) ' |x|=' num2str(normx)])
407     assert(normx<20,'solution exploding')
408     tbs = tb0+(0:0.033:0.2);
```

Figure 4.3: macro-scale view of heterogeneous advection-diffusion PDE along a (periodic) channel obtained via the patch scheme.



```

409     spmd
410         xb0 = codistributed(xb0,patches.codist);
411         xbs = RK2mesoPatch(tbs,xb0,[],patches);
412     end%spmd
413     xbs=reshape(xbs{1},length(tbs),[]);
414 end%function

```

Fin.

4.1.4 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 (4.2) at each point in the interior of a patch, output in ct . The heterogeneous advects and diffusivities, $u_i(y_j)$ and $\kappa_i(y_{j+1/2})$, have previously been merged and stored in the one array `patches.cs` (2D).

```

22 function ct = chanDispMicro(t,c,p)
23     [nx,ny,~,~]=size(c); % micro-grid points in patches
24     ix = 2:nx-1;           % x interior points in a patch
25     dx = diff(p.x(2:3)); % x space step
26     dy = 2/ny;             % y space step
27     ct = nan+c;            % preallocate output array
28     pcs = reshape(p.cs,nx-1,[],2);

```

Compute the cross-channel flux using ‘ghost’ nodes at channel boundaries, so that the flux is zero at $y = \pm 1$ either because the boundary values are replicated so the differences are zero, or because the diffusivities in `cs` are zero at the channel boundaries.

```
38     ydif = pcs(ix,1:2:end,2) ...
39         .*(c(ix,[1:end end],:,:)-c(ix,[1 1:end],:,:))/dy;
```

Now evaluate advection-diffusion time derivative (4.2). Could use upwind advection and no longitudinal diffusion, or, as here, centred advection and diffusion.

```
48     ct(ix,:,:,:) = (ydif(:,2:end,:,:)-ydif(:,1:end-1,:,:))/dy ...
49         + diff(pcs(:,2:2:end,2).*diff(c))/dx^2 ...
50         - p.Pe*pcs(ix,2:2:end,1).*(c(ix+1,:,:,:)-c(ix-1,:,:,:))/(2*dx);
51 end% function
```

4.2 rotFilmSpmd: simulation of a 2D shallow water flow on a rotating heterogeneous substrate

Section contents

4.2.1	Simulate heterogeneous advection-diffusion	139
4.2.2	Plot the solution	142
4.2.3	microBurst function for Projective Integration	143
4.2.4	rotFilmMicro(): 2D shallow water flow on a rotating heterogeneous substrate	144

As an example application, consider the flow of a shallow layer of fluid on a solid flat rotating substrate, such as in spin coating (Wilson et al. 2000, Oron et al. 1997, §II.K, e.g.) or large-scale shallow water waves (Dellar & Salmon 2005, Hereman 2009, e.g.). Let $\vec{x} = (x, y)$ parametrise location on the rotating substrate, and let the fluid layer have thickness $h(\vec{x}, t)$ and move with depth-averaged horizontal velocity $\vec{v}(\vec{x}, t) = (u, v)$. We take as given (with its simplified physics) that the (non-dimensional) governing set of PDEs is the nonlinear system (Bunder & Roberts 2018, eq. (1), e.g.)

$$\frac{\partial h}{\partial t} = -\nabla \cdot (h\vec{v}), \quad (4.3a)$$

$$\frac{\partial \vec{v}}{\partial t} = \begin{bmatrix} -b & f \\ -f & -b \end{bmatrix} \vec{v} - (\vec{v} \cdot \nabla) \vec{v} - g\nabla h + \vec{\nabla} \cdot (\nu \vec{\nabla} \vec{v}), \quad (4.3b)$$

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 4.5).

For the microscale computation, Section 4.2.4 discretises the PDEs (4.3) in space with x, y -spacing $\delta x, \delta y$.

Choose one of four cases:

- theCase=1 is corresponding code without parallelisation (in this toy problem it is much the quickest because there is no expensive communication);
- theCase=2 illustrates that RK2mesoPatch invokes spmd computation if parallel has been configured.
- theCase=3 shows how users explicitly invoke spmd-blocks around the time integration.

- `theCase=4` invokes projective integration for long-time simulation via short bursts of the micro-computation, bursts done within `spmd`-blocks for parallel computing.

First, clear all to remove any existing globals, old composites, etc—although a parallel pool persists. Then choose the case.

```
71 clear all
72 theCase = 1
```

Set micro-scale bed drag (array 1) and diffusivity (arrays 2–3) to be a heterogeneous log-normal factor with specified period: modify the strength of the heterogeneity by the coefficient of `randn` from zero to perhaps one: coefficient 0.3 appears a good moderate value.

```
82 mPeriod = 5
83 bnu = shiftdim([1 0.5 0.5], -1) ...
84 .*exp(0.3*randn([mPeriod mPeriod 3]));
```

Configure the patch scheme with these choices of domain, patches, size ratios—here each patch is square in space. In Cases 1–2, set `patches` information to be global so the info can be used without being explicitly passed as arguments.

```
96 if theCase<=2, global patches, end
```

In Case 4, double the size of the domain and use more separated patches accordingly, to maintain the spatial microscale grid spacing to be 0.055. Here use fourth order edge-based coupling between patches. Choose the parallel option if not Case 1, which invokes `spmd`-block internally, so that field variables become *distributed* across cpus.

```
108 nSubP = 2+mPeriod
109 nPatch = 9
110 ratio = 0.2+0.2*(theCase<4)
111 Len = 2*pi*(1+(theCase==4))
112 disp('**** Setting configPatches2')
113 patches = configPatches2(@rotFilmMicro, [0 Len], nan ...
114 , nPatch, 4, ratio, nSubP, 'EdgyInt', true ...
115 , 'hetCoeffs', bnu, 'parallel', (theCase>1) );
```

When using parallel, any additional parameters to `patches`, such as physical parameters for the microcode, must be set within a `spmd` block (because `patches` is a co-distributed structure). Here set frequency of substrate rotation, and strength of gravity.

```
125 f = 5, g = 1
126 if theCase==1, patches.f = f; patches.g = g;
127 else      spmd, patches.f = f; patches.g = g; end
128 end
```

4.2.1 Simulate heterogeneous advection-diffusion

Set initial conditions of a simulation as shown in [Figure 4.4](#). Here the initial condition is a (periodic) quasi-Gaussian in h and zero velocity \vec{v} , with additive

random perturbations.

```
141 disp('**** Set initial condition and test dhuv0dt =')
142 if theCase==1
```

When not parallel processing, invoke the usual operations. Here add a random noise to the velocity field, but keep $h(x, y, 0)$ smooth as shown by [Figure 4.4](#). The `shiftdim(...,-1)` moves the given row-vector of coefficients into the third dimension to become coefficients of the fields (h, u, v) , respectively.

```
153 huv0 = shiftdim([0.5 0 0],-1) ...
154 . *exp(-cos(patches.x)/2-cos(patches.y));
155 huv0 = huv0+0.1*shiftdim([0 1 1],-1).*rand(size(huv0));
156 dhuv0dt = patchSys2(0,huv0);
```

With parallel, we must use an `spmd`-block for computations: there is no difference in Cases 2–4 here. Also, we must sometimes explicitly tell functions how to distribute some initial condition arrays over the cpus. Now `patchSys2` does not invoke `spmd` so higher level code must, as here. Even if `patches` is global, inside an `spmd`-block we *must* pass `patches` explicitly as a parameter to `patchSys2`.

```
170 else, spmd
171     huv0 = shiftdim([0.5 0 0],-1) ...
172         . *exp(-cos(patches.x)/2-cos(patches.y));
173     huv0 = huv0+0.1*rand(size(huv0),patches.codist);
174     dhuv0dt = patchSys2(0,huv0,patches)
175     end%spmd
176 end%if theCase
```

Integrate in time, either via the automatic `ode23` or via `RK2mesoPatch` which reduces communication between patches. By default, `RK2mesoPatch` does ten micro-steps for each specified meso-step in `ts`. For stability: with noise up to 0.3, need micro-steps less than 0.0003; with noise 1, need micro-steps less than 0.0001.

```
201 warning('Integrating system in time, wait a minute')
202 ts=0:0.003:0.3;
```

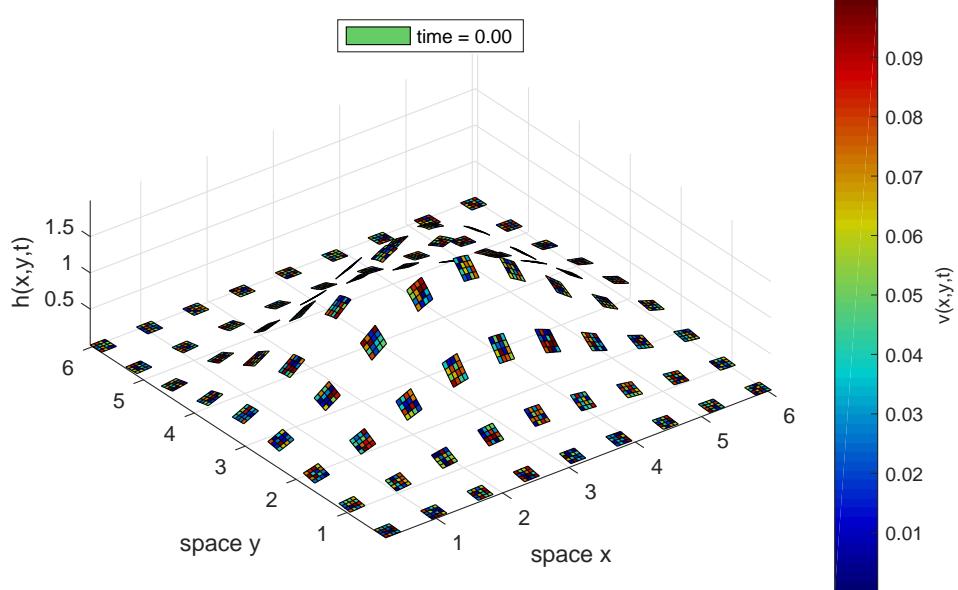
Go to the selected case.

```
208 switch theCase
```

1. For non-parallel, we could use `RK2mesoPatch` as indicated below, but instead choose to use standard `ode23` as here `patchSys2` accesses patch information via global `patches`. For post-processing, reshape each and every row of the computed solution to the correct array size—namely that of the initial condition.

```
220 case 1
221 %    tic,[huvs,uerrs] = RK2mesoPatch(ts,huv0);toc
222 [ts,huvs] = ode23(@patchSys2,[0 4],huv0(:));
223 huvs=reshape(huvs,[length(ts) size(huv0)]);
```

Figure 4.4: initial field $h(x, y, 0)$ of the patch scheme applied to the heterogeneous, shallow water, rotating substrate, PDE (4.3). The micro-scale sub-patch colour displays the initial y -direction velocity field $v(x, y, 0)$. Figure 4.5 plots the roughly smooth field values at time $t = 6$. In this example the patches are relatively large, ratio 0.4, for visibility.



2. In the second case, RK2mesoPatch detects a parallel patch code has been requested, but has only one cpu worker, so it auto-initiates an `spmd`-block for the integration. Both this and the next case return *composite* results, so just keep one version of the results.

```
235 case 2
236     huvs = RK2mesoPatch(ts,huv0);
237     huvs = huvs{1};
```

3. In this third case, a user could merge this explicit `spmd`-block with the previous one that sets the initial conditions.

```
246 case 3,spmd
247     huvs = RK2mesoPatch(ts,huv0,[],patches);
248 end%spmd
249 huvs = huvs{1};
```

4. In this fourth case, use Projective Integration (PI). Currently the PI is done serially, with parallel `spmd`-blocks only invoked inside function `aBurst()` (Section 4.2.3) 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 4.2.3) in order to provide shaped initial states, and to provide the patch information.

```
264 case 4
265     microBurst = @(tb0,xb0,bT) ...
```

```

266      aBurst(tb0 ,reshape(xb0,size(huv0)) ,patches);
267      ts = 0:0.1:1
268      huvs = PIRK2(microBurst,ts,gather(huv0(:)));
269      huvs = reshape(huvs,[length(ts) size(huv0)]);
End the four cases.

276 end%switch theCase

```

4.2.2 Plot the solution

Optionally set to save some plots to file.

```
287 if 0, global OurCf2eps, OurCf2eps=true, end
```

Animate the computed solution field over time

```
293 figure(1), clf, colormap(0.8*jet)
```

First get the x -coordinates and omit the patch-edge values from the plot (because they are not here interpolated).

```

300 if theCase==1, x = patches.x;
301     y = patches.y;
302 else, spmd
303     x = gather( patches.x );
304     y = gather( patches.y );
305 end%spmd
306 x = x{1}; y = y{1};
307 end
308 x([1 end],:,:,(:,:,,:)) = nan;
309 y(:,:,1,[1 end],:,:, :) = nan;

```

Draw the field values as a patchy surface evolving over 100–200 time steps.

```
316 nTimes = length(ts)
317 for l = 1:ceil(nTimes/200):nTimes
```

At each time, squeeze sub-patch data fields into three 4D arrays, permute to get all the x/y -variations in the first/last two dimensions, and then reshape to 2D.

```

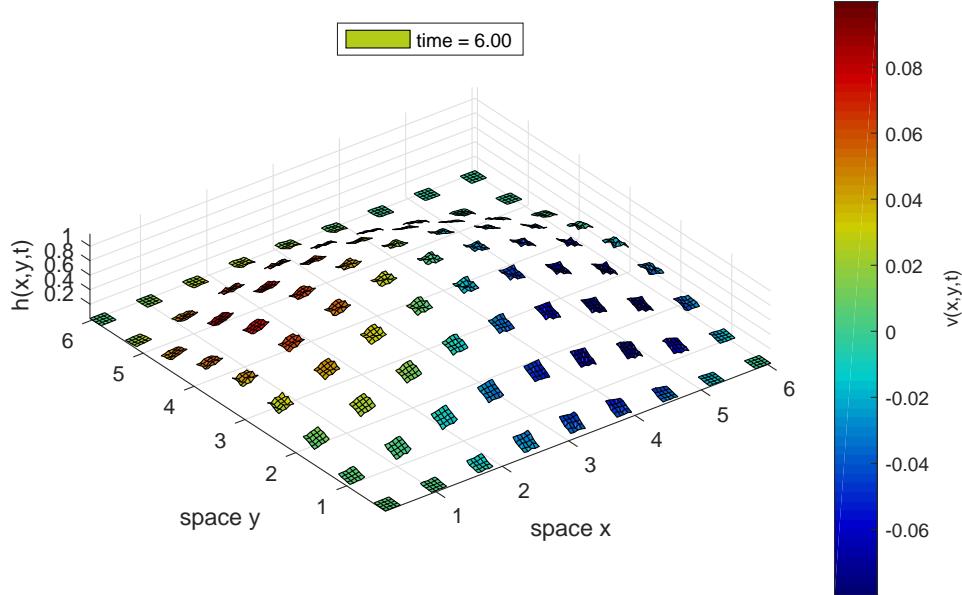
325 h = reshape( permute( squeeze( ...
326     huvs(l,:,:,:,1,1,:,:,:) ) ,[1 3 2 4]) ,numel(x),numel(y));
327 u = reshape( permute( squeeze( ...
328     huvs(l,:,:,:,2,1,:,:,:) ) ,[1 3 2 4]) ,numel(x),numel(y));
329 v = reshape( permute( squeeze( ...
330     huvs(l,:,:,:,3,1,:,:,:) ) ,[1 3 2 4]) ,numel(x),numel(y));

```

Draw surface of each patch, to show both micro-scale and macro-scale variation in space. Colour the surface according to the velocity v in the y -direction.

```
338 if l==1
339     hp = surf(x(:,y(:,h',v'));
```

Figure 4.5: 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 (4.3) with heterogeneous factors log-normal, here distributed $\exp[\mathcal{N}(0, 1)]$.



```

340     axis([0 Len 0 Len 0 max(h(:))])
341     c = colorbar; c.Label.String = 'v(x,y,t)';
342     legend(['time = ' num2str(ts(1),'%4.2f')] ...
343             , 'Location','north')
344     axis equal
345     xlabel('space x'), ylabel('space y'), zlabel('h(x,y,t)')
346     ifOurCf2eps([mfilename 't0'])
347     disp('**** pausing, press blank to begin animation')
348     pause
349 else
350     hp.ZData = h'; hp.CData = v';
351     legend(['time = ' num2str(ts(1),'%4.2f')])
352     pause(0.1)
353 end
370 end%for over time
371 ifOurCf2eps([mfilename 'tFin'])

```

Finish the animation loop, and optionally save the final plot to file, [Figure 4.5](#).

4.2.3 microBurst function for Projective Integration

Projective Integration stability appears to require bursts longer than 0.01. Each burst is done in parallel processing. Here use RK2mesoPatch to take meso-steps, each with default ten micro-steps so the micro-scale step is 0.0003. With macro-step 0.1, these parameters usually give stable projective integration.

```

388 function [tbs,xbs] = aBurst(tb0,xb0,patches)
389     normx=max(abs(xb0(:)));
390     disp(['* aBurst t=' num2str(tb0) ' |x|=' num2str(normx)])
391     assert(normx<20,'solution exploding')
392     tbs = tb0+(0:0.003:0.015);
393     spmd
394         xb0 = codistributed(xb0,patches.codist);
395         xbs = RK2mesoPatch(tbs,xb0,[],patches);
396     end%spmd
397     xbs=reshape(xbs{1},length(tbs),[]);
398 end%function

```

Fin.

4.2.4 rotFilmMicro(): 2D shallow water flow on a rotating heterogeneous substrate

This function codes the heterogeneous shallow water flow (4.3) 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 3.14), computes the time derivatives (4.3) at each point in the interior of a patch, output in `huvt`. The heterogeneous bed drag and diffusivities, b_{ij} and ν_{ij} , have previously been merged and stored in the array `patches.cs` (2D × 3): herein `patches` is named `p`.

```

24 function huvt = rotFilmMicro(t,huv,p)
25 [nx,ny,~]=size(huv); % micro-grid points in patches
26 i = 2:nx-1;           % x interior points in a patch
27 j = 2:ny-1;           % y interior points in a patch
28 dx = diff(p.x(2:3)); % x space step
29 dy = diff(p.y(2:3)); % y space step
30 huvt = nan+huv;      % preallocate output array

```

Set indices of fields in the arrays. Need to store different diffusivity values for the x , y -directions as they are evaluated at different points in space.

```

38 h=1; u=2; v=3;
39 b=1; nux=2; nuy=3;

```

Use a staggered micro-grid so that $h(i,j) = h_{ij}$, $u(i,j) = u_{i+1/2,j}$, and $v(i,j) = v_{i,j+1/2}$. We need the following to interpolate some quantities to other points on the staggered micro-grid. But the first two statements fill-in two needed corner values because they are not (currently) interpolated by `patchEdgeInt2()`.

```

51 huv(1,ny,u,:,:,:) = huv(2,ny,u,:,:,:)+huv(1,ny-1,u,:,:,:);
52             -huv(2,ny-1,u,:,:,:);
53 huv(nx,1,v,:,:,:) = huv(nx,2,v,:,:,:)+huv(nx-1,1,v,:,:,:);
54             -huv(nx-1,2,v,:,:,:);
55 v4u = (huv(i,j-1,v,:,:,:)+huv(i+1,j,v,:,:,:));
56             +huv(i,j,v,:,:,:)+huv(i+1,j-1,v,:,:,:))/4;

```

```

57 u4v = (huv(i,j+1,u,:,:,:)+huv(i-1,j,u,:,:,:))/4;
58     +huv(i,j,u,:,:,:)+huv(i-1,j+1,u,:,:,:))/4;
59 h2u = (huv(2:nx,:,h,:,:,:)+huv(1:nx-1,:,h,:,:,:))/2;
60 h2v = (huv(:,2:ny,h,:,:,:)+huv(:,1:ny-1,h,:,:,:))/2;

```

Evaluate conservation of mass PDE (4.3a) (needing averages of h at half-grid points):

```

67 huvt(i,j,h,:,:,:) = ...
68 - (h2u(i,j ,:,:,:,:).*huv(i ,j,u,:,:,:)) ...
69 - h2u(i-1,j ,:,:,:,:).*huv(i-1,j,u,:,:,:)/dx ...
70 - (h2v(i,j ,:,:,:,:).*huv(i,j ,v,:,:,:)) ...
71 - h2v(i,j-1,:,:,:,:).*huv(i,j-1,v,:,:,:))/dy ;

```

Evaluate the x -direction momentum PDE (4.3b) (needing to interpolate component v to u -points):

```

79 huvt(i,j,u,:,:,:) = ...
80 - p.cs(i,j,b).*huv(i,j,u,:,:,:)+ p.f.*v4u ...
81 - huv(i,j,u,:,:,:).*(huv(i+1,j,u,:,:,:)-huv(i-1,j,u,:,:,:))/(2*dx) ...
82 - v4u.* (huv(i,j+1,u,:,:,:)-huv(i,j-1,u,:,:,:))/(2*dy) ...
83 - p.g*(huv(i+1,j,h,:,:,:)-huv(i,j,h,:,:,:))/dx ...
84 + diff(p.cs(:,j,nux).*diff(huv(:,j,u,:,:,:),[],1),[],1)/dx^2 ...
85 + diff(p.cs(i,:,nuy).*diff(huv(i,:,u,:,:,:),[],2),[],2)/dy^2 ;

```

Evaluate the y -direction momentum PDE (4.3b) (needing to interpolate component u to v -points):

```

93 huvt(i,j,v,:,:,:) = ...
94 - p.cs(i,j,b).*huv(i,j,v,:,:,:)- p.f.*u4v ...
95 - u4v.* (huv(i+1,j,v,:,:,:)-huv(i-1,j,v,:,:,:))/(2*dx) ...
96 - huv(i,j,v,:,:,:).*(huv(i,j+1,v,:,:,:)-huv(i,j-1,v,:,:,:))/(2*dy) ...
97 - p.g*(huv(i,j+1,h,:,:,:)-huv(i,j,h,:,:,:))/dy ...
98 + diff(p.cs(:,j,nux).*diff(huv(:,j,v,:,:,:),[],1),[],1)/dx^2 ...
99 + diff(p.cs(i,:,nuy).*diff(huv(i,:,v,:,:,:),[],2),[],2)/dy^2 ;
100 end% function

```

4.3 homoDiff31spmd: computational homogenisation of a 1D dispersion via parallel simulation on small 3D patches of heterogeneous diffusion

Section contents

4.3.1	Simulate heterogeneous diffusion	147
4.3.2	Plot the solution	149
4.3.3	<code>microBurst</code> function for Projective Integration	150

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 3.25](#).

Choose one of four cases:

- `theCase=1` is corresponding code without parallelisation (in this toy problem it is much the quickest because there is no expensive communication);
- `theCase=2` for minimising coding by a user of `spmd`-blocks;
- `theCase=3` is for users happier to explicitly invoke `spmd`-blocks.
- `theCase=4` invokes projective integration for long-time simulation via short bursts of the micro-computation, bursts done within `spmd`-blocks for parallel computing.

First, clear all to remove any existing globals, old composites, etc—although a parallel pool persists. Then choose the case.

```
48 clear all
49 theCase = 1
```

Set micro-scale heterogeneity with various spatial periods in the three directions.

```
57 mPeriod = [4 3 2] %1+randperm(3)
58 cHetr = exp(0.3*randn([mPeriod 3]));
59 cHetr = cHetr*mean(1./cHetr(:))
```

Configure the patch scheme with some arbitrary choices of domain, patches, size ratios—here each patch is a unit cube in space. Choose some random order of interpolation. Set `patches` information to be global so the info can be used for Case 1 without being explicitly passed as arguments. Choose the parallel option if not Case 1, which invokes `spmd`-block internally, so that field variables become *distributed* across cpus.

```

73 if any(theCase==[1 2]), global patches, end
74 nSubP=mPeriod+2
75 nPatch=[9 1 1]
76 ratio=0.3
77 Len=nPatch(1)/ratio
78 ordCC=2*randi([0 3])
79 disp('**** Setting configPatches3')
80 patches = configPatches3(@heteroDiff3,[0 Len 0 1 0 1], nan ...
81 , nPatch, ordCC, [ratio 1 1], nSubP, 'EdgyInt',true ...
82 , 'hetCoeffs',cHetr , 'parallel',(theCase>1) );

```

4.3.1 Simulate heterogeneous diffusion

Set initial conditions of a simulation as shown in [Figure 4.6](#).

```

92 disp('**** Set initial condition and testing du0dt =')
93 if theCase==1

```

Without parallel processing, invoke the usual operations.

```

99 u0 = exp( -(patches.x-Len/2).^2/Len ...
100 -patches.y.^2/2-patches.z.^2 );
101 u0 = u0.* (1+0.2*rand(size(u0)));
102 du0dt = patchSys3(0,u0);

```

With parallel, must use an `spmd`-block for computations: there is no difference in cases 2–4 here. Also, we must sometimes explicitly code how to distribute some new arrays over the cpus. Now `patchSys3` does not invoke `spmd` so higher level code must, as here. Even if `patches` is global, inside `spmd`-block we must pass it explicitly as a parameter to `patchSys3`.

```

115 else, spmd
116     u0 = exp( -(patches.x-Len/2).^2/Len ...
117 -patches.y.^2/2-patches.z.^2/4 );
118     u0 = u0.* (1+0.2*rand(size(u0),patches.codist));
119     du0dt = patchSys3(0,u0,patches);
120     end%spmd
121 end%if theCase

```

Integrate in time. Use non-uniform time-steps for fun, and to show more of the initial rapid transients.

Alternatively, use `RK2mesoPatch` which reduces communication between patches, recalling that, by default, `RK2mesoPatch` does ten micro-steps for each specified step in `ts`. For unit cube patches, need micro-steps less than about 0.004 for stability.

```

144 warning('Integrating system in time, wait patiently')
145 ts=0.4*linspace(0,1,21).^2;

```

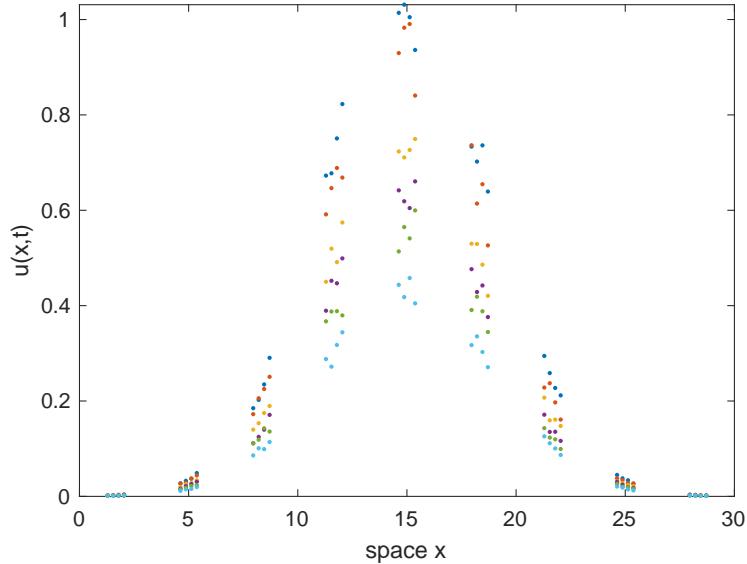
Go to the selected case.

```

151 switch theCase

```

Figure 4.6: 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 4.7 plots the nearly smooth field values at time $t = 0.4$.



1. For non-parallel, we could use `RK2mesoPatch` as indicated below, but instead choose to use standard `ode23` as here `patchSys3` accesses patch information via global `patches`. For post-processing, reshape each and every row of the computed solution to the correct array size—that of the initial condition.

```

163 case 1
164 % [us,uerrs] = RK2mesoPatch(ts,u0);
165 [ts,us] = ode23(@patchSys3,ts,u0(:));
166 us=reshape(us,[length(ts) size(u0)]);

```

2. In the second case, `RK2mesoPatch` detects a parallel patch code has been requested, but has only one cpu worker, so it auto-initiates an `spmd`-block for the integration. Both this and the next case return *composite* results, so just keep one version of the results.

```

178 case 2
179 us = RK2mesoPatch(ts,u0);
180 us = us{1};

```

3. In this third case, a user could merge this explicit `spmd`-block with the previous one that sets the initial conditions.

```

189 case 3,spmd
190 us = RK2mesoPatch(ts,u0,[],patches);
191 end%spmd
192 us = us{1};

```

4. In this fourth case, use Projective Integration (PI) over long times (`PIRK4` also works). Currently the PI is done serially, with parallel

spmd-blocks only invoked inside function `aBurst()` ([Section 4.3.3](#)) 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 4.3.3](#)) in order to provide shaped initial states, and to provide the patch information.

```

210 case 4
211     microBurst = @(tb0,xb0,bT) ...
212         aBurst(tb0 ,reshape(xb0,size(u0)) ,patches);
213     ts = 0:3:51
214     us = PIRK2(microBurst,ts,gather(u0(:)));
215     us = reshape(us,[length(ts) size(u0)]);
222 end%switch theCase

```

End the four cases.

4.3.2 Plot the solution

Optionally save some plots to file.

```
233 if 0, global OurCf2eps, OurCf2eps=true, end
```

Animate the solution field over time. Since the spatial domain is long in x and thin in y, z , just plot field values as a function of x .

```

241 figure(1), clf
242 if theCase==1
243     x = reshape( patches.x(2:end-1,:,:,:) ,[],1);
244 else, spmd
245     x = reshape(gather( patches.x(2:end-1,:,:,:) ),[],1);
246 end%spmd
247 x = x{1};
248 end

```

For every time step draw the field values as dots and pause for a short display.

```
255 nTimes = length(ts)
256 for l = 1:length(ts)
```

At each time, squeeze interior point data into a 4D array, permute to get all the x -variation in the first two dimensions, and reshape into x -variation for each and every (y, z) .

```
265 u = reshape( permute( squeeze( ...
266     us(1,2:end-1,2:end-1,2:end-1,:) ) ,[1 4 2 3]) ,numel(x),[]);
```

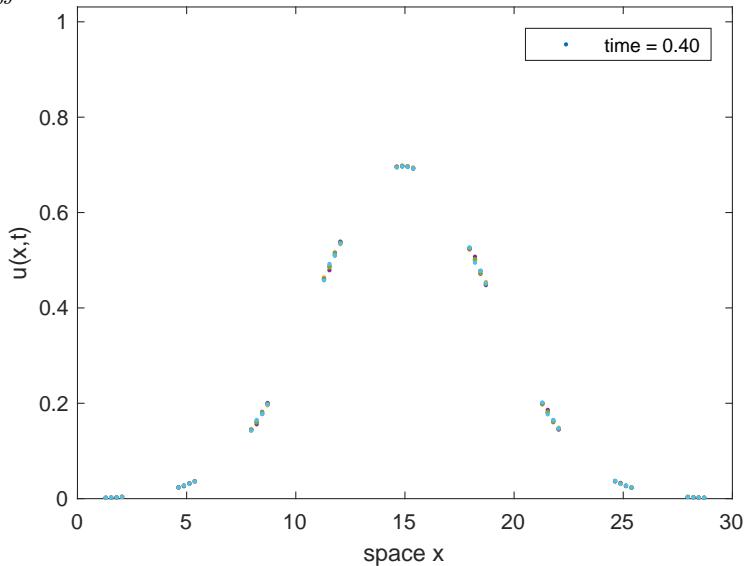
Draw point data to show spread at each cross-section, as well as macro-scale variation in the long space direction.

```
273 if l==1
274     hp = plot(x,u,'.');

```

² Curiously, `PIG()` appears to suffer unrecoverable instabilities with its variable step size!

Figure 4.7: final field $u(x, y, z, 0.4)$ of the patch scheme applied to a heterogeneous diffusion PDE.



```

275 axis([0 Len 0 max(u(:))])
276 xlabel('space x'), ylabel('u(x,y,z,t)')
277 ifOurCf2eps([mfilename 't0'])
278 legend(['time = ' num2str(ts(1),'%4.2f')])
279 disp('**** pausing, press blank to animate')
280 pause
281 else
282 for p=1:size(u,2), hp(p).YData=u(:,p); end
283 legend(['time = ' num2str(ts(1),'%4.2f')])
284 pause(0.1)
285 end

```

Finish the animation loop, and optionally output the final plot, Figure 4.7.

```

298 end%for over time
299 ifOurCf2eps([mfilename 'tFin'])

```

4.3.3 microBurst function for Projective Integration

Projective Integration stability seems to need bursts longer than 0.2. Here take ten meso-steps, each with default ten micro-steps so the micro-scale step is 0.002. With macro-step 3, these parameters usually give stable projective integration (but not always).

```

315 function [tbs,xbs] = aBurst(tb0,xb0,patches)
316     normx=max(abs(xb0(:)));
317     disp(['aBurst t = ' num2str(tb0) ' |x| = ' num2str(normx)])
318     assert(normx<10,'solution exploding')
319     tbs = tb0+(0:0.02:0.2);
320     spmd
321         xb0 = codistributed(xb0,patches.codist);

```

```
322      xbs = RK2mesoPatch(tbs,xb0,[],patches);  
323      end%spmd  
324      xbs=reshape(xbs{1},length(tbs),[]);  
325  end%function
```

Fin.

4.4 RK2mesoPatch()

This is a Runge–Kutta, 2nd order, integration of a given deterministic system of ODEs on patches. It invokes meso-time updates of the patch-edge values in order to reduce interpolation costs, and uses a linear variation in edge-values over the meso-time-step (Bunder et al. 2016, case $Q = 2$). This function is aimed primarily for large problems executed on a computer cluster to markedly reduce expensive communication between computers.

If using within projective integration, it appears quite tricky to get all the time-steps chosen appropriately. One has to choose times for: the micro-scale time-step, the meso-time interval between communications, the longer meso-time burst length, and the macro-scale integration time-step.

```
27 function [xs,errs] = RK2mesoPatch(ts,x0,nMicro,patches)
28 if nargin<4, global patches, end
```

Input

- `patches.fun()` is a function such as `dxdt=fun(t,x,patches)` that computes the right-hand side of the ODE $d\vec{x}/dt = \vec{f}(t, \vec{x})$ where \vec{x} is a vector/array, t is a scalar, and the result \vec{f} is a correspondingly sized vector/array.
- `x0` is an vector/array of initial values at the time `ts(1)`.
- `ts` is a vector of meso-scale times to compute the approximate solution, say in \mathbb{R}^ℓ for $\ell \geq 2$.
- `nMicro`, optional, default 10, is the number of micro-time-steps taken for each meso-scale time-step.
- `patches` struct set by `configPatchesn` and provided as either as parameter, or as a global variable.

Output

- `xs`, 5/7/9D (depending upon `nD`) array of length $\ell \times \dots$ of approximate solution vector/array at the specified times. But, if using parallel computing via `spmd`, then `xs` is a *composite* 5/7/9D array, so outside of an `spmd`-block access a single copy of the array via `xs{1}`. Similarly for `errs`.
- `errs`, column vector in \mathbb{R}^ℓ of local error estimate for the step from t_{k-1} to t_k .

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