

# Equation-Free function toolbox for Matlab/Octave

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December 13, 2018

## Abstract

This ‘equation-free toolbox’ facilitates the computer-assisted analysis of complex, multiscale systems. Its aim is to enable microscopic simulators to perform system level tasks and analysis. The methodology bypasses the derivation of macroscopic evolution equations by using only short bursts of microscale simulations which are often the best available description of a system (Kevrekidis & Samaey 2009, Kevrekidis et al. 2004, 2003, e.g.). This suite of functions should empower users to start implementing such methods—but so far we have only just started.

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# 1 Introduction

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**Users** Place this toolbox’s folder in a path searched by MATLAB/Octave. Then read the subsection that documents the function of interest.

**Blackbox scenario** Assume that a researcher/practitioner has a detailed and *trustworthy* computational simulation of some problem of interest. The simulation may be written in terms of micro-positional coordinates  $\vec{x}_i(t)$  in ‘space’ at which there are micro-field variable values  $\vec{u}_i(t)$  for indices  $i$  in some (large) set of integers and for time  $t$ . In lattice problems the positions  $\vec{x}_i$  would be fixed in time (unless employing a moving mesh on the microscale); in particle problems the positions would evolve. The positional coordinates are  $\vec{x}_i \in \mathbb{R}^d$  where for spatial problems integer  $d = 1, 2, 3$ , but it may be more when solving for a distribution of velocities, or pore sizes, or trader’s beliefs, etc. The mirco-field variables could be in  $\mathbb{R}^p$  for any  $p = 1, 2, \dots, \infty$ .

Further, assume that the computational simulation is too expensive over all the desired spatial domain  $\mathbb{X} \subset \mathbb{R}^d$ . Thus we aim a toolbox to simulate only on macroscale distributed patches.

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

MATLAB appears the obvious choice for a first version since it is widespread, reasonably efficient, supports various parallel modes, and development costs are reasonably low. Further it is built on BLAS and LAPACK so potentially the cache and superscalar CPU are well utilised. Let’s develop functions

that work for both MATLAB/Octave. Appendix A outlines some details for contributors.

## 2 Overview of major functions and example scripts

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### 2.1 Projective integration of deterministic ODEs

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This section provides some good projective integration functions (Gear & Kevrekidis 2003a,b, Givon et al. 2006, e.g.). The goal is to enable computationally expensive dynamic simulations to be run over long time scales. Perhaps start by looking at Section 3.1 which codes the introductory example of a long time simulation of the Michaelis–Menton multiscale system of differential equations.

**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 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 the long-time scale a variant of a standard numerical method to simulate the emergent dynamics of the complex system. Each function has standardised inputs and outputs.

### 2.1.1 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  $y(t)$ :

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

As illustrated in [Figure 2](#), 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  $\epsilon$ .

### 2.1.2 PIRK2(): projective integration of second order accuracy

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

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

**Input** If there are no input arguments, then this function applies itself to the Michaelis–Menton example: see the code in [Section 3.2.1](#) as a basic template of how to use.

- `solver()`, a function that produces output from the user-specified code for microscale simulation.

```
[tOut, xOut] = solver(tStart, xStart, tSim)
```

- Inputs: `tStart`, the start time of a burst of simulation; `xStart`, the row  $n$ -vector of the starting state; `tSim`, the total time to simulate in the burst.
- Outputs: `tOut`, the column vector of solution times; and `xOut`, an array in which each *row* contains the system state at corresponding times.
- `bT`, a scalar, the minimum amount of time needed for simulation of the microsolver to relax the fast variables to the slow manifold.
- `tSpan` is an  $\ell$ -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`: they are included in the simulation and output, and often represent boundaries in space fields.

**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(solver, bT, tSpan, x0)`.

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

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

- **xms**, optional, is an  $L \times n$  array of the corresponding microscale states—this data is an accurate simulation of the state and may help visualise more details of the solution.
- **rm**, optional, a struct containing the ‘remaining’ applications of the microsolver 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 in general resemble the true dynamics.

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

### 2.1.3 Example: PI using Runge–Kutta macrosolvers

This script is a demonstration of the **PIRK()** schemes, that use a Runge–Kutta macrosolver, applied to a simple linear system with some slow and fast directions.

### 2.1.4 PIG(): Projective Integration with a General macrosolver

This is an approximate Projective Integration scheme in which the macrosolver is given by any user-specified scheme. Unlike the **PIRK** functions,

**PIG()** cannot estimate the slow vector field at the times expected by any user-specified scheme, but instead provides an estimate of the slow vector field at a slightly different time, after an application of the microsolver. Consequently **PIG()** will incur an additional global error term proportional to the burst length of the microscale simulator. For that reason, **PIG()** should be used with very stiff problems, in which the burst length of the microsolver can be short, or with the ‘constraint defined manifold’ based microsolver provided by **cdmc()**, that attempts to project the variables onto the slow manifold without affecting the time.

14 `function [t, x, tms, xms, svf] = PIG(solver,bT,macro,IC)`

The inputs and outputs are necessarily a little different to the two **PIRK2** functions.

## Input

- **solver()**, a function that produces output from the user-specified code for micro-scale simulation. Usage:  
`[tout,xout] = solver(t_in,x_in,tSim)` Inputs: **t\_in**, the initialisation time; **x\_in**  $\in \mathbb{R}^n$ , the initial state; **tSim**, the time to simulate for.  
 Outputs: **tout**, the vector of solution times, and **xout**, the corresponding states.
- **bT**, a scalar, the minimum amount of time thought needed for integration of the microsolver to relax the fast variables to the slow manifold.

The remaining inputs to **PIG()** set the solver and parameters used for macroscale simulation.

- **macro**, a struct holding information about the macrosolver.
  - **macro.solver()**, the numerical method that the user wants to apply on a slow time scale. The solver should be formatted as a standard numerical method in Matlab/Octave that is called as

`[t_out,x_out] = solver(f,tspan,IC)` for an ordinary differential equation  $\frac{dx}{dt} = f(t, x)$ , vector of input times `tspan` and initial condition `IC`. The function `f(t,x)` is not an input for `PIG()` but will instead be estimated by PI.

- `macro.tspan`, a vector of times at which the user requests output, of which the first element is always the initial time. If `macro.solver` can adaptively select time steps (e.g. `ode45`), then `tspan` can consist of an initial and final time only.
- `IC`, an  $n$ -vector of initial values at the time `tspan(1)`.

**Output** Standard usage is to output only macrosolver information, with the following usage:

```
x = PIG(micro,macro,IC)
```

- `x`, a cell array. `x{1}`, an  $\ell$ -vector of times at which PI produced output. `x{2}`, an  $\ell \times n$  array of the approximate solution vector. Each row corresponds to an element of `x{1}`.

It is also possible to return the microsolver applications called by the PI method in executing the user-defined macrosolver. Much of this microscale data will not be an accurate solution of the system, but rather will consist of simulations used to relax the fast variables close to the slow manifold in the process of executing a single macroscale time step.

```
[x,xm] = PIRK4(micro,tspan,IC)
```

- `xm`, a cell array containing the output of all applications of the microsolver. `xm{1}` is an  $L$  dimensional column vector containing times; `xm{2}` is an  $L \times n$  array of the corresponding microsolver output.

```
[x,xm,dx] = PIRK4(micro,tspan,IC)
```

- `dx`, a cell array containing the PI estimates of the slow vector field. `dx{1}` is an  $\ell$  dimensional column vector containing all times at which

the PI scheme extrapolated along microsolver data to form a macrostep.  $\mathbf{dx}\{2\}$  is an  $\ell \times n$  array containing the estimated slow vector field.

### 2.1.5 Example 2: PI using General macrosolvers

In this example the PI-General scheme is applied to a singularly perturbed ordinary differential equation. The aim is to allow a standard non-stiff numerical integrator, e.g. `ode45()`, to be applied to a stiff problem on a slow, long time scale.

### 2.1.6 Minor functions

**cdmc()** `cdmc()` iteratively applies the microsolver and then projects backwards in time to the initial conditions. 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.

#### Input

- **solver**, a black box microsolver suitable for PI. See any of `PIRK2()`, `PIRK4()`, `PIG()` for a description of `solver()`.
- **t**, an initial time
- **x**, an initial state
- **T**, a time period to apply `solver()` for

#### Output

- **tout**, a vector of times. `tout(end)` will equal `t`.
- **xout**, an array of state estimates produced by `solver()`.

**bbgen()** `bbgen()` is a simple function that takes a standard numerical method and produces a black box solver of the type required by the PI schemes.

```
12 function bb = bbgen(solver,f,dt)
```

## Input

- `solver`, a standard numerical solver for ordinary differential equations
- `f`, a function  $f(t,x)$  taking time and state inputs
- `dt`, a time step suitable for simulation with `f`

**Output** `bb = bb( $t_{in}, x_{in}, T$ )` a ‘black box’ microsolver that initialises at  $(t_{in}, x_{in})$  and simulates forward a duration  $T$ .

### 2.1.7 Explore: PI using constraint-defined manifold computing

In this example the PI-General scheme is applied to a singularly perturbed ordinary differential equation in which the time scale separation is not too strong. The resulting simulation is not accurate. In parallel, we run the same scheme but with `cdmc()` used as a wrapper for the microsolver. This second implementation successfully replicates the true dynamics.

### 2.1.8 PIRK4(): projective integration of fourth order accuracy

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

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

The inputs and outputs are standardised with `PIRK2()`.

## Input

- `solver()`, a function that produces output from the user-specified code for microscale simulation.

```
[tOut, xOut] = solver(tStart, xStart, tSim)
```

- Inputs: `tStart`, the start time of a burst of simulation; `xStart`, the row  $n$ -vector of the starting state; `tSim`, the total time to simulate in the burst.
- Outputs: `tOut`, the column vector of solution times; and `xOut`, an array in which each *row* contains the system state at corresponding times.
- `bT`, a scalar, the minimum amount of time needed for simulation of the microsolver to relax the fast variables to the slow manifold.
- `tSpan` is an  $\ell$ -vector of times at which the user requests output, of which the first element is always the initial time. `PIRK4()` does not use adaptive time stepping; the macroscale time steps are (nearly) the steps between elements of `tSpan`.
- `x0` is an  $n$ -vector of initial values at the initial time `tSpan(1)`. Elements of `x0` may be `NaN`: they are included in the simulation and output, and often represent boundaries in space fields.

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

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

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

- **tms**, optional, is an  $L$  dimensional column vector containing microscale times of burst simulations, each burst separated by **NaN**;
- **xms**, optional, is an  $L \times n$  array of the corresponding microscale states—this data is an accurate simulation of the state and may help visualise more details of the solution.
- **rm**, optional, a struct containing the ‘remaining’ applications of the microsolver 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 in general resemble the true dynamics.

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

## 2.2 Patch scheme for given microscale discrete space system

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The patch scheme applies to spatio-temporal systems where the spatial domain is larger than what can be computed in reasonable time. Then one may simulate 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 spatial discrete system is to be on a lattice such as obtained from finite difference approximation of a PDE. Usually continuous in time.

**Quick start** For an example, see Sections 4.1.1 and 4.7.1 for basic code that uses the provided functions to simulate Burgers' PDE and a nonlinear 'diffusion' PDE.

## 2.2.1 `configPatches1()`: configures spatial patches in 1D

Makes the struct `patches` for use by the patch/gap-tooth time derivative function `patchSmooth1()`. Section 4.1.1 lists an example of its use.

```
17 function configPatches1(fun,Xlim,BCs,nPatch,ordCC,ratio,nSubP,nEdge)
18 global patches
```

**Input** If invoked with no input arguments, then executes an example of simulating Burgers' PDE—see [Section 4.1.1](#) for the example code.

- **fun** is the name of the user function, `fun(t,u,x)`, that computes time derivatives (or time-steps) of quantities on the patches.
- **Xlim** give the macro-space domain of the computation: patches are equi-spaced over the interior of the interval  $[Xlim(1), Xlim(2)]$ .
- **BCs** somehow will define the macroscale boundary conditions. Currently, **BCs** is ignored and the system is assumed macro-periodic in the domain.
- **nPatch** is the number of equi-spaced spaced patches.
- **ordCC** is the ‘order’ of interpolation across empty space of the macroscale mid-patch values to the edge of the patches for inter-patch coupling: currently must be in  $\{-1, 0, \dots, 8\}$ .
- **ratio** (real) is the ratio of the half-width of a patch to the spacing of the patch mid-points: so  $ratio = \frac{1}{2}$  means the patches abut; and  $ratio = 1$  is overlapping patches as in holistic discretisation.
- **nSubP** is the number of equi-spaced microscale lattice points in each patch. Must be odd so that there is a central lattice point.
- **nEdge** is, for each patch, the number of edge values set by interpolation at the edge regions of each patch. May be omitted. The default is one (suitable for microscale lattices with only nearest neighbour interactions).

**Output** The *global* struct **patches** is created and set with the following components.

- **.fun** is the name of the user’s function `fun(u,t,x)` that computes the time derivatives (or steps) on the patchy lattice.
- **.ordCC** is the specified order of inter-patch coupling.
- **.alt** 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` are the `ordCC`-vector of weights for the inter-patch interpolation onto the right and left edges (respectively) with patch:macroscale ratio as specified.
- `.x` is `nSubP × nPatch` array of the regular spatial locations  $x_{ij}$  of the microscale grid points in every patch.
- `.nEdge` is, for each patch, the number of edge values set by interpolation at the edge regions of each patch.

## 2.2.2 `patchCoreSmooth1()`: interface to time integrators

To simulate in time with spatial patches we often need to interface a users time derivative function with time integration routines such as `ode15s` or `PIRK2`. This function provides an interface. Either the sub-patch structure is *smooth* so that the patch centre-values are sensible macroscale variables, or the user chooses to average over a *core* of values in the centre of each patch with these averages providing sensible macroscale variables (no core averaging corresponds to a core of size one). Patch edge values are determined by macroscale interpolation of the patch-centre values or core-averaged values. Communicate patch-design variables to this function using the previously established global struct `patches`.

```
28 function dudt=patchCoreSmooth1(t,u)
29 global patches
```

### Input

- `u` is a vector of length `nSubP · nPatch · nVars` where there are `nVars` field values at each of the points in the `nSubP × nPatch` grid.
- `t` is the current time to be passed to the user's time derivative function.
- `patches` a struct set by `configPatches1()` with the following information used here.

- `.fun` is the name of the user's function `fun(t,u,x)` that computes the time derivatives on the patchy lattice. The array `u` has size `nSubP × nPatch × nVars`. Time derivatives must be computed into the same sized array, but herein the patch edge values are overwritten by zeros.
- `.x` is `nSubP × nPatch` array of the spatial locations  $x_{ij}$  of the microscale grid points in every patch. Currently it *must* be an equi-spaced lattice on both macro- and micro-scales.

## Output

- `dudt` is `nSubP · nPatch · nVars` vector of time derivatives, but with patch edge values set to zero.

### 2.2.3 `patchEdgeInt1()`: sets edge values from interpolation over the macroscale

Couples 1D patches across 1D space by computing their edge values from macroscale interpolation. Consequently a spatially discrete system could be integrated in time via the patch or gap-tooth scheme (Roberts & Kevrekidis 2007). Assumes that the sub-patch structure or core averages are *smooth* so are sensible macroscale variables, and patch edge values are determined by macroscale interpolation of the patch-centre values or patch cores. Communicate patch-design variables via the global struct `patches`.

```
22 function u=patchCoreEdgeInt1(u)
23 global patches
```

## Input

- `u` is a vector of length `nSubP · nPatch · nVars` where there are `nVars` field values at each of the points in the `nSubP × nPatch` grid.

- **patches** a struct set by `configPatches1()` which includes the following.
  - `.x` is  $nSubP \times nPatch$  array of the spatial locations  $x_{ij}$  of the microscale grid points in every patch. Currently it *must* be an equi-spaced lattice on both macro- and micro-scales.
  - `.ordCC` is order of interpolation, currently in  $\{0, 2, 4, 6, 8\}$ .
  - `.alt` in  $\{0, 1\}$  is one for staggered grid (alternating) interpolation.
  - `.Cwtsr` and `.Cwtsl`

## Output

- `u` is  $nSubP \times nPatch \times nVars$  2/3D array of the fields with edge values set by interpolation.

### 2.2.4 BurgersExample: simulate Burgers' PDE on patches

[Figure 7](#) shows an example simulation in time generated by the patch scheme function applied to Burgers' PDE. This code similarly applies the Equation-Free functions to a microscale space-time map ([Figure 8](#)), a map that happens to be derived as a micro-scale space-time discretisation of Burgers' PDE. Then this example applies projective integration to simulate further in time.

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

1. `configPatches1`
2. `burgerBurst`  $\leftrightarrow$  `patchSmooth1`  $\leftrightarrow$  `burgersMap`
3. process results

### 2.2.5 HomogenisationCoreExample: simulate heterogeneous diffusion in 1D on patches

Figure 11 and Figure 12 show example simulations in time generated by the patch scheme function applied to heterogeneous diffusion without and with an ensemble average, respectively. 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 minus the number of points in the core is an even multiple of the microscale periodicity (assuming the microscale periodicity is periodic on the macroscale domain).

We present two different methods of obtaining a macroscale solution. One method uses the given heterogeneous diffusion, which produces a solution which is rough at the microscale. The other method constructs an ensemble of heterogeneous diffusion and produces an ensemble average solution which is smooth at the microscale.

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

1. configPatches1
2. ode15s  $\leftrightarrow$  patchSmooth1  $\leftrightarrow$  heteroDiff
3. process results

### 2.2.6 waterWaveExample: simulate a water wave PDE on patches

Figure 17 shows an example simulation in time generated by the patch scheme function applied to a simple wave PDE. The inter-patch coupling is realised by spectral interpolation to the patch edges of the mid-patch values.

This approach, based upon the differential equations coded in Section 4.6.2, may be adapted by a user to a wide variety of 1D wave and near-wave systems. For example, the differential equations of Section 4.6.3 describes the nonlinear microscale simulator of the nonlinear shallow water wave PDE

derived from the Smagorinski model of turbulent flow (Cao & Roberts 2012, 2016a).

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

Makes the struct `patches` for use by the patch/gap-tooth time derivative function `patchSmooth2()`. Section 4.7.1 lists an example of its use.

```
17 function configPatches2(fun,Xlim,BCs,nPatch,ordCC,ratio,nSubP,nEdge)
18 global patches
```

**Input** If invoked with no input arguments, then executes an example of simulating a nonlinear diffusion PDE relevant to the lubrication flow of a thin layer of fluid—see Section 4.7.1 for the example code.

- `fun` is the name of the user function, `fun(t,u,x,y)`, that computes time derivatives (or time-steps) of quantities on the patches.
- `Xlim` array/vector giving the macro-space domain of the computation: patches are equi-spaced over the interior of the rectangle  $[Xlim(1), Xlim(2)] \times [Xlim(3), Xlim(4)]$ : if of length two, then use the same interval in both directions, otherwise `Xlim(1:4)` give the interval in each direction.
- `BCs` somehow will define the macroscale boundary conditions. Currently, `BCs` is ignored and the system is assumed macro-periodic in the domain.
- `nPatch` determines the number of equi-spaced spaced patches: if scalar, then use the same number of patches in both directions, otherwise `nPatch(1:2)` give the number in each direction.
- `ordCC` is the ‘order’ of interpolation across empty space of the macroscale mid-patch values to the edge of the patches for inter-patch coupling: currently must be in {0}.
- `ratio` (real) is the ratio of the half-width of a patch to the spacing of the patch mid-points: so `ratio = 1/2` means the patches abut; and

**ratio** = 1 would be overlapping patches as in holistic discretisation: if scalar, then use the same ratio in both directions, otherwise **ratio(1:2)** give the ratio in each direction.

- **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. Must be odd so that there is a central lattice point.
- **nEdge** is, for each patch, the number of edge values set by interpolation at the edge regions of each patch. May be omitted. The default is one (suitable for microscale lattices with only nearest neighbours. interactions).

**Output** The *global* struct **patches** is created and set with the following components.

- **.fun** is the name of the user's function **fun(u,t,x,y)** that computes the time derivatives (or steps) on the patchy lattice.
- **.ordCC** is the specified order of inter-patch coupling.
- **.alt** 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**-vector of weights for the inter-patch interpolation onto the right and left edges (respectively) with patch:macroscale ratio as specified.
- **.x** is **nSubP(1) × nPatch(1)** array of the regular spatial locations  $x_{ij}$  of the microscale grid points in every patch.
- **.y** is **nSubP(2) × nPatch(2)** array of the regular spatial locations  $y_{ij}$  of the microscale grid points in every patch.
- **.nEdge** is, for each patch, the number of edge values set by interpolation at the edge regions of each patch.

### 2.2.8 patchSmooth2(): interface to time integrators

To simulate in time with spatial patches we often need to interface a users time derivative function with time integration routines such as `ode15s` or `PIRK2`. This function provides an interface. It assumes that the sub-patch structure is *smooth* so that the patch centre-values are sensible macroscale variables, and patch edge values are determined by macroscale interpolation of the patch-centre values. Communicate patch-design variables to this function via the previously established global struct `patches`.

```
23 function dudt=patchSmooth2(t,u)
24 global patches
```

#### Input

- `u` is a vector of length `prod(nSubP) · prod(nPatch) · nVars` where there are `nVars` 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,x,y)` that computes the time derivatives on the patchy lattice. The array `u` has size `nSubP(1) × nSubP(2) × nPatch(1) × nPatch(2) × nVars`. Time derivatives must be computed into the same sized array, but herein the patch edge values are overwritten by zeros.
  - `.x` is `nSubP(1) × nPatch(1)` array of the spatial locations  $x_{ij}$  of the microscale grid points in every patch. Currently it *must* be an equi-spaced lattice on both macro- and micro-scales.
  - `.y` is similarly `nSubP(2) × nPatch(2)` array of the spatial locations  $y_{ij}$  of the microscale grid points in every patch. Currently it *must* be an equi-spaced lattice on both macro- and micro-scales.

## Output

- `dudt` is `prod(nSubP) · prod(nPatch) · nVars` vector of time derivatives, but with patch edge values set to zero.

### 2.2.9 `patchEdgeInt2()`: sets 2D patch edge values from 2D macroscale interpolation

Couples 2D patches across 2D space by computing their edge values via macroscale interpolation. Assumes that the sub-patch structure is *smooth* so that the patch centre-values are sensible macroscale variables, and patch edge values are determined by macroscale interpolation of the patch-centre values. Communicate patch-design variables via the global struct `patches`.

```
21 function u=patchEdgeInt2(u)
22 global patches
```

## Input

- `u` is a vector of length `nx · ny · Nx · Ny · nVars` where there are `nVars` field values at each of the points in the `nx × ny × Nx × Ny` grid on the `Nx × Ny` array of patches.
- `patches` a struct set by `configPatches2()` which includes the following information.
  - `.x` is `nx × Nx` array of the spatial locations  $x_{ij}$  of the microscale grid points in every patch. Currently it *must* be an equi-spaced lattice on both macro- and micro-scales.
  - `.y` is similarly `ny × Ny` array of the spatial locations  $y_{ij}$  of the microscale grid points in every patch. Currently it *must* be an equi-spaced lattice on both macro- and micro-scales.
  - `.ordCC` is order of interpolation, currently only `{0}`.
  - `.Cwtsr` and `.Cwtsl`—not yet used

## Output

- **u** is **nx × ny × Nx × Ny × nVars** array of the fields with edge values set by interpolation.

### 2.2.10 wave2D: example of a wave on patches in 2D

For  $u(x, y, t)$ , test and simulate the simple wave PDE in 2D space:

$$\frac{\partial^2 u}{\partial t^2} = \nabla^2 u .$$

This script shows one way to get started: a user's script may have the following three steps (arrows indicate function recursion).

1. configPatches2
2. ode15s integrator  $\leftrightarrow$  patchSmooth2  $\leftrightarrow$  wavePDE
3. process results

### 3 Projective integration of deterministic ODEs

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This section provides some good projective integration functions ([Gear & Kevrekidis 2003a,b](#), [Givon et al. 2006](#), e.g.). The goal is to enable computationally expensive dynamic simulations to be run over long time scales. Perhaps start by looking at [Section 3.1](#) which codes the introductory example of a long time simulation of the Michaelis–Menton multiscale system of differential equations.

**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 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 the long-time scale a variant of a standard numerical method to simulate the emergent dynamics of the complex system. Each function has standardised inputs and outputs.

## Main functions

- Projective Integration by second or fourth order Runge–Kutta, [PIRK2\(\)](#) and [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 solver, `PIG()`. This function enables a Projective Integration implementation of any solver with macroscale time steps. It does not matter whether the solver is a standard Matlab or Octave algorithm, or one supplied by the user. As explored in later examples, `PIG()` should only be used in very stiff systems.

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

## Minor functions

- ‘Constraint-defined manifold computing’, `cdmc()`. This helper function, based on the method introduced in ?, iteratively applies the microsolver and projects the output backwards in time. The result is to constrain the fast variables close to the slow manifold, without advancing the current time by the duration of an application of the microsolver. This function can be used to reduce errors related to the simulation length of the microsolver in either the `PIRK` or `PIG` functions. In particular, it enables `PIG()` to be used on problems that are not particularly stiff.
- Black box microsolver generator, `bbgen()`. This simple function takes as input a standard solver with a recommended time step for microscale simulation, and returns a ‘black box’ microsolver for the Projective Integration functions.

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

### 3.1 egPIMM: Example projective integration of Michaelis–Menton kinetics

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

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

As illustrated in [Figure 2](#), 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  $\epsilon$ .

#### 3.1.1 Invoke projective integration

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

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

First, [Section 3.1.2](#) encodes the computation of bursts of the Michaelis–Menten system in a function `MMburst()`. Second, here set macroscale times of computation and interest into vector `ts`. Then, invoke Projective Integration with `PIRK2()` applied to the burst function, say using bursts of simulations of length  $2\epsilon$ , and starting from the initial condition for the Michaelis–Menten system of  $(x(0), y(0)) = (1, 0)$  (off the slow manifold).

```
48 ts = 0:6
49 xs = PIRK2(@MMburst, 2*epsilon, ts, [1;0])
50 plot(ts,xs,'o:')
51 xlabel('time t'), legend('x(t)', 'y(t)')
52 pause(1)
```

Figure 1: Michaelis–Menton enzyme kinetics simulated with the projective integration of `PIRK2()`: macroscale samples.

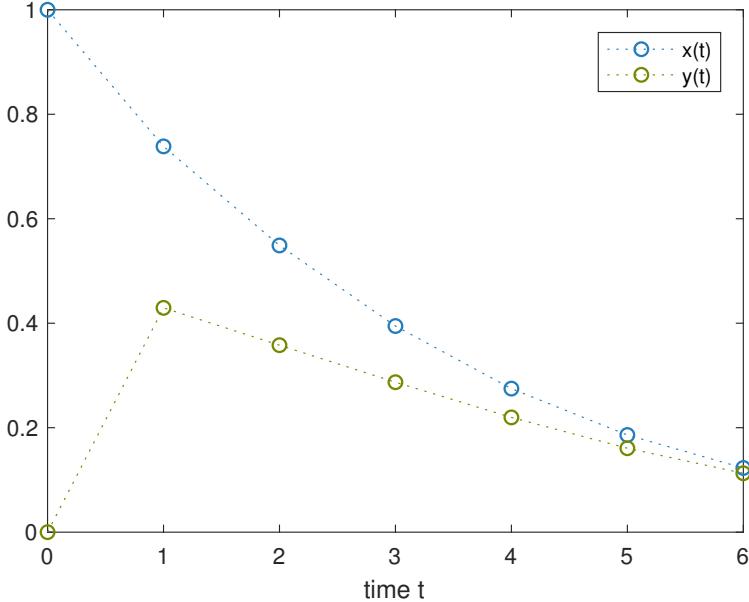


Figure 1 plots the macroscale results showing the long time decay of the Michaelis–Menton system on the slow manifold.

**Optional: 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 1). To see the initial transient attraction to the slow manifold we plot some microscale data in Figure 2. Two further output variables provide this microscale burst information.

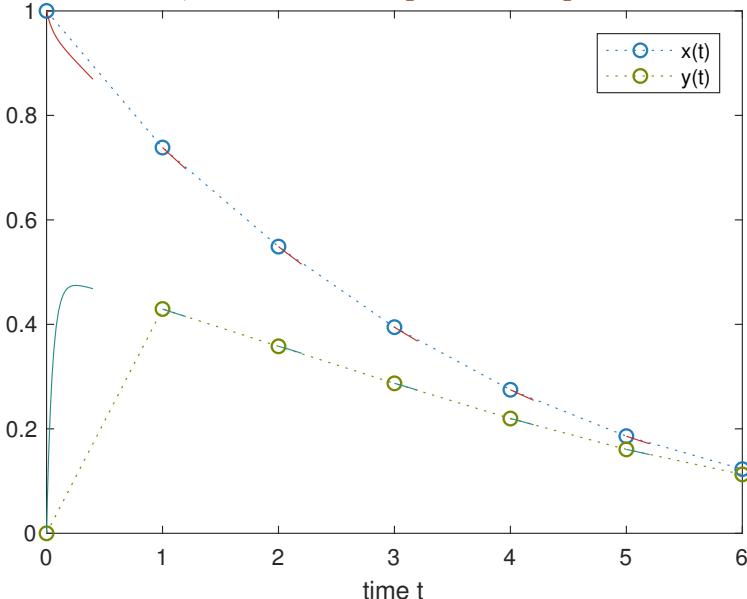
```

77 [xs,tMicro,xMicro] = PIRK2(@MMburst, 2*epsilon, ts, [1;0]);
78 figure, plot(ts,xs,'o:',tMicro,xMicro)
79 xlabel('time t'), legend('x(t)', 'y(t)')
80 pause(1)

```

Figure 2 plots the macroscale and microscale results—also showing that the

Figure 2: 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.



initial burst is by default twice as long. Observe the slow variable  $x(t)$  is also affected by the initial transient which indicates that other schemes which ‘freeze’ slow variables are less accurate.

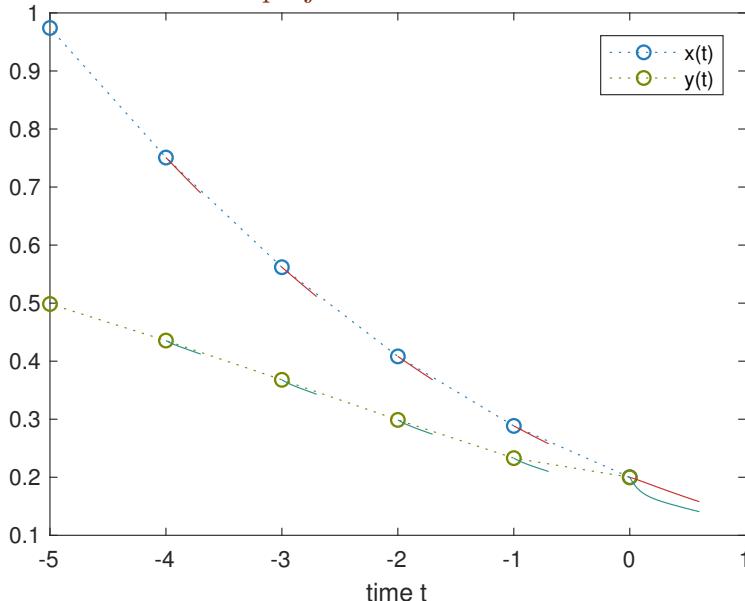
**Optional: simulate backwards in time** Figure 3 shows that projective integration even simulates backwards in time along the slow manifold using short forward bursts. Such backwards macroscale simulations succeed despite the fast variable  $y(t)$ , when backwards in time, being viciously unstable. However, backwards integration appears to need longer bursts, here  $3\epsilon$ .

```

110 ts = 0:-1:-5
111 [xs,tMicro,xMicro] = PIRK2(@MMburst, 3*epsilon, ts, 0.2*[1;1]);
112 figure, plot(ts, xs, 'o:', tMicro, xMicro)

```

Figure 3: Michaelis–Menton enzyme kinetics simulated backwards with the projective integration of PIRK2(): the microscale bursts show the short forward simulations used to project backwards in time at  $\epsilon = 0.1$ .



```
113 xlabel('time t'), legend('x(t)', 'y(t)')
```

### 3.1.2 Code a burst of Michaelis–Menton enzyme kinetics

Say use `ode23()` to integrate a burst of the differential equations for the Michaelis–Menton enzyme kinetics. Code differential equations in function `dMMdt` with variables  $x = \mathbf{x}(1)$  and  $y = \mathbf{x}(2)$ . For the given start time `ti`, and start state `xi`, `ode23()` integrates the differential equations for a burst time of `bT`, and return the simulation data.

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

```

143      1/epsilon*( x(1)-(x(1)+1)*x(2) )];
144      [ts, xs] = ode23(dMMdt, [ti ti+bT], xi);
145 end

```

## 3.2 PIRK2(): projective integration of second order accuracy

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

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

**Input** If there are no input arguments, then this function applies itself to the Michaelis–Menton example: see the code in [Section 3.2.1](#) as a basic template of how to use.

- **solver()**, a function that produces output from the user-specified code for microscale simulation.

**[tOut, xOut] = solver(tStart, xStart, tSim)**

- Inputs: **tStart**, the start time of a burst of simulation; **xStart**, the row  $n$ -vector of the starting state; **tSim**, the total time to simulate in the burst.
- Outputs: **tOut**, the column vector of solution times; and **xOut**, an array in which each *row* contains the system state at corresponding times.
- **bT**, a scalar, the minimum amount of time needed for simulation of the microsolver to relax the fast variables to the slow manifold.
- **tSpan** is an  $\ell$ -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`: they are included in the simulation and output, and often represent boundaries in space fields.

**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(solver,bT,tSpan,x0)`.

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

- `tms`, optional, is an  $L$  dimensional column vector containing microscale times of burst simulations, each burst separated by `NaN`;
- `xms`, optional, is an  $L \times n$  array of the corresponding microscale states—this data is an accurate simulation of the state and may help visualise more details of the solution.
- `rm`, optional, a struct containing the ‘remaining’ applications of the microsolver 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 in general resemble the true dynamics.

- `svf`, optional, a struct containing the Projective Integration estimates of the slow vector field.
  - `svf.t` is a  $2\ell$  dimensional column vector containing all times at

which the Projective Integration scheme is extrapolated along microsolver data to form a macrostep.

- `svf.dx` is a  $2\ell \times n$  array containing the estimated slow vector field.

### 3.2.1 If no arguments, then execute an example

```
113 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  $y(t)$  (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  $x(0) = 1$  and  $y(0) = 0$ , the following code computes and plots a solution over time  $0 \leq t \leq 6$  for parameter  $\epsilon = 0.05$  using bursts of length  $3\epsilon$ .

```
130 epsilon = 0.05
131 ts = 0:6
132 [x,tms,xms,rm,svf] = PIRK2(@MMburst, 3*epsilon, ts, [1;0]);
133 figure, plot(ts,x,'o:',tms,xms)
134 title('Projective integration of Michaelis--Menton enzyme kinetics')
135 xlabel('time t'), legend('x(t)', 'y(t)')
```

Upon finishing execution of the example, exit this function.

```
141 return
142 end%if no arguments
```

**Example function code for a burst of ODEs** Integrate a burst of length  $bT$  of the ODEs for the Michaelis–Menton enzyme kinetics at parameter  $\epsilon$  inherited from above. Code ODEs in function `dMMdt` with variables

$x = \mathbf{x}(1)$  and  $y = \mathbf{x}(2)$ . Starting at time  $\mathbf{ti}$ , and state  $\mathbf{xi}$  (row), here code the midpoint integration scheme.

```

156 function [ts, xs] = MMBurst(ti, xi, bT)
157     dMMdt = @t,x) [ -x(1)+(x(1)+0.5)*x(2)
158                     1/epsilon*( x(1)-(x(1)+1)*x(2) ) ];
159     ts = linspace(ti,ti+bT,ceil(bT*5/epsilon))';
160     dt = ts(2)-ts(1);
161     xs = nan(length(ts),length(xi));
162     xs(1,:) = xi;
163     for j = 1:length(ts)-1
164         xMidpoint = xs(j,:)+dt/2*dMMdt(ts(j),xs(j,:)).';
165         xs(j+1,:) = xs(j,:)+dt*dMMdt(ts(j)+dt/2,xMidpoint).';
166     end
167 end

```

### 3.2.2 The projective integration code

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

```

181 nT=length(tSpan);
182 x=nan(nT,length(x0));

```

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

```

190 nArgs=nargout();
191 saveMicro = (nArgs>1);
192 saveFullMicro = (nArgs>3);
193 saveSvf = (nArgs>4);

```

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

```
206 x0 = reshape(x0,1,[]);
207 [relax_t,relax_x0] = solver(tSpan(1),x0,bT);
```

Use the end point of the microsolver as the initial conditions.

```
215 tSpan(1) = tSpan(1)+bT;
216 x(1,:)=relax_x0(end,:);
```

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

```
226 if saveMicro
227     tms = cell(nT,1);
228     xms = cell(nT,1);
229     tms{1} = reshape(relax_t,[],1);
230     xms{1} = relax_x0;
231     if saveFullMicro
232         rm.t = cell(nT,1);
233         rm.x = cell(nT,1);
234         if saveSvf
235             svf.t = nan(2*nT-2,1);
236             svf.dx = nan(2*nT-2,length(x0));
237         end
238     end
239 end
```

### Loop over the macroscale time steps

```
247 for jT = 2:nT
248     T = tSpan(jT-1);
```

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

```
256     if 2*abs(bT)>=abs(tSpan(jT)-T) & bT*(tSpan(jT)-T)>0
257         [t1,xm1] = solver(T, x(jT-1,:), tSpan(jT)-T);
```

```

258      x(jT,:) = xm1(end,:);
259      t2=nan; xm2=nan(1,size(xm1,2));
260      dx1=xm2; dx2=xm2;
261  else

```

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

```

272      [t1,xm1] = solver(T, x(jT-1,:), bT);
273      del = t1(end)-t1(end-1);

```

Check for round-off error.

```

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

```

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

```

292      Dt = tSpan(jT)-T-bT;
293      dx1 = (xm1(end,:)-xm1(end-1,:))/del;

```

Project along **dx1** to form an intermediate approximation of **x**; run another application of the microsolver and form a second estimate of the slow vector field.

```

303      xint = xm1(end,:)+(Dt-bT)*dx1;
304      [t2,xm2] = solver(T+Dt, xint, bT);
305      del = t2(end)-t2(end-1);
306      dx2 = (xm2(end,:)-xm2(end-1,:))/del;

```

Check for round-off error.

```

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

```

```
314     warning(['significant round-off error in 2nd projection at T=' n
315     end
```

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

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

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

```
331     end
```

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

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

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

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

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

```
362     if saveSvf
363         svf.t(2*jT-3:2*jT-2) = [t1(end); t2(end)];
364         svf.dx(2*jT-3:2*jT-2,:) = [dx1; dx2];
365     end
366
367     end
```

Terminate the main loop:

```
373 end
```

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

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

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

```
390 if saveMicro
391     tms = cell2mat(tms);
392     xms = cell2mat(xms);
393     if saveFullMicro
394         rm.t = cell2mat(rm.t);
395         rm.x = cell2mat(rm.x);
396     end
397 end
```

### 3.2.3 If no output specified, then plot simulation

```
405 if nArgs==0
406     figure, plot(tSpan,x,'o:')
407     title('Projective Simulation with PIRK2')
408 end
415 end
```

This concludes `PIRK2()`.

## 3.3 Example: PI using Runge–Kutta macrosolvers

This script is a demonstration of the `PIRK()` schemes, that use a Runge–Kutta macrosolver, applied to a simple linear system with some slow and fast directions.

Clear workspace and set a seed.

```
12 clear
13 rng(1)
```

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

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

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

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

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

```
35 f = gen_linear_system(7,3,fastband,slowband);
```

Set the time step size and total integration time of the microsolver.

```
41 dt = 0.001;
```

```
42 bT = 0.05;
```

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

```
49 solver='fe';
```

(Other options: '`rk2`' for second order Runge–Kutta, '`rk4`' for fourth order, or any Matlab/Octave integrator such as '`ode45`'.)

A crucial part of the PI philosophy is that it does not assume anything about the microsolver. For this reason, the microsolver must be a ‘black box’, which is run by specifying an initial time and state, and a duration to simulate for. All the details of the microsolver must be set by the user. We generate and save a black box microsolver.

```
62 bbm = bbgen(solver,f,dt);
63 solver = bbm;
```

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

```
70 tSpan=0: 1 : 30;
71 IC = linspace(-10,10,10);
```

We implement the PI scheme, saving the coarse states in `x`, the ‘trusted’ applications of the microsolver in `xmicro`, and the additional applications of the microsolver in `xrmicro`. Note that the second and third outputs are optional and do not need to be set.

```
80 [x, tms, xms, rm] = PIRK4(solver, bT, tSpan, IC);
```

For verification, we also compute the trajectories using a standard solver.

```
86 [tt,ode45x] = ode45(f,tSpan([1,end]),IC);
```

Figure 4 plots the output.

```
99 tmsr = rm.t; xmsr = rm.x;
100 clf()
101 hold on
102 PI_sol=plot(tSpan,x,'bo');
103 std_sol=plot(tt,ode45x,'r');
104 plot(tms,xms,'k.');
105 plot(tmsr,xmsr,'g.');
106 legend([PI_sol(1),std_sol(1)],'PI Solution',...
107 'Standard Solution','Location','NorthWest')
108 xlabel('Time');
109 ylabel('State');
```

Save plot to a file.

```
115 set(gcf,'PaperPosition',[0 0 14 10])
116 print('-depsc2','PIRK')
```

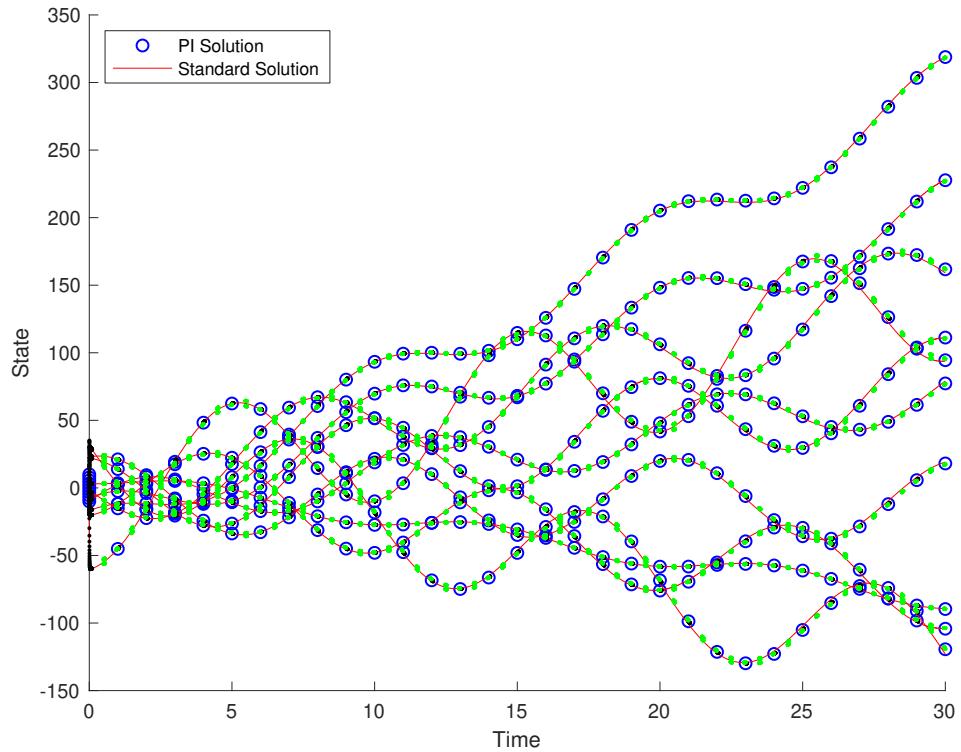


Figure 4: Demonstration of PIRK4(). From initial conditions, the system rapidly transitions to an attracting invariant manifold. The PI solution accurately tracks the evolution of the variables over time while requiring only a fraction of the computations of the standard solver.

### 3.4 PIG(): Projective Integration with a General macrosolver

This is an approximate Projective Integration scheme in which the macrosolver is given by any user-specified scheme. Unlike the `PIRK` functions, `PIG()` cannot estimate the slow vector field at the times expected by any user-specified scheme, but instead provides an estimate of the slow vector field at a slightly different time, after an application of the microsolver. Consequently `PIG()` will incur an additional global error term proportional to the burst length of the microscale simulator. For that reason, `PIG()` should be used with very stiff problems, in which the burst length of the microsolver can be short, or with the ‘constraint defined manifold’ based microsolver provided by `cdmc()`, that attempts to project the variables onto the slow manifold without affecting the time.

<sup>14</sup> `function [t, x, tms, xms, svf] = PIG(solver,bT,macro,IC)`

The inputs and outputs are necessarily a little different to the two `PIRK2` functions.

#### Input

- `solver()`, a function that produces output from the user-specified code for micro-scale simulation. Usage:  
`[tout,xout] = solver(t_in,x_in,tSim)` Inputs: `t_in`, the initialisation time;  $x_{in} \in \mathbb{R}^n$ , the initial state; `tSim`, the time to simulate for.  
 Outputs: `tout`, the vector of solution times, and `xout`, the corresponding states.
- `bT`, a scalar, the minimum amount of time thought needed for integration of the microsolver to relax the fast variables to the slow manifold.

The remaining inputs to `PIG()` set the solver and parameters used for macroscale simulation.

- **macro**, a struct holding information about the macrosolver.
  - **macro.solver()**, the numerical method that the user wants to apply on a slow time scale. The solver should be formatted as a standard numerical method in Matlab/Octave that is called as `[t_out,x_out] = solver(f,tspan,IC)` for an ordinary differential equation  $\frac{dx}{dt} = f(t,x)$ , vector of input times **tspan** and initial condition **IC**. The function **f(t,x)** is not an input for **PIG()** but will instead be estimated by PI.
  - **macro.tspan**, a vector of times at which the user requests output, of which the first element is always the initial time. If **macro.solver** can adaptively select time steps (e.g. `ode45`), then **tspan** can consist of an initial and final time only.
- **IC**, an  $n$ -vector of initial values at the time **tspan(1)**.

**Output** Standard usage is to output only macrosolver information, with the following usage:

```
x = PIG(micro,macro,IC)
```

- **x**, a cell array. **x{1}**, an  $\ell$ -vector of times at which PI produced output. **x{2}**, an  $\ell \times n$  array of the approximate solution vector. Each row corresponds to an element of **x{1}**.

It is also possible to return the microsolver applications called by the PI method in executing the user-defined macrosolver. Much of this microscale data will not be an accurate solution of the system, but rather will consist of simulations used to relax the fast variables close to the slow manifold in the process of executing a single macroscale time step.

```
[x,xm] = PIRK4(micro,tspan,IC)
```

- **xm**, a cell array containing the output of all applications of the microsolver. **xm{1}** is an  $L$  dimensional column vector containing times; **xm{2}** is an  $L \times n$  array of the corresponding microsolver output.

```
[x,xm,dx] = PIRK4(micro,tspan,IC)
```

- **dx**, a cell array containing the PI estimates of the slow vector field. **dx{1}** is an  $\ell$  dimensional column vector containing all times at which the PI scheme extrapolated along microsolver data to form a macrostep. **dx{2}** is an  $\ell \times n$  array containing the estimated slow vector field.

The main body of the function now follows.

Get microscale and macroscale information from inputs, and compute the number of time steps at which output is expected.

```
69  tspan = macro.tspan;
70  csolve = macro.solver;
71  nT=length(tspan)-1;
72  sIC = length(IC);
```

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

```
79  nArgs=nargout();
80  saveMicro = (nArgs>1);
81  saveSvf = (nArgs>2);
```

Run a first application of the microsolver on the initial conditions. This is done in addition to the microsolver in the main loop, because the initial conditions are often far from the attracting slow manifold.

```
90  IC = reshape(IC,[],1);
91  [relax_t,relax_IC] = solver(tspan(1),IC,bT);
```

Update the initial time.

```
98  tspan(1) = tspan(1)+bT;
```

Allocate cell arrays for times and states for any of the outputs requested by the user. If saving information, then record the first application of the microsolver. Note that it is unknown a priori how many applications of the microsolver will be required; this code may be run more efficiently if the correct number is used in place of **N+1** as the dimension of the cell arrays.

```

107 if saveMicro
108     tms=cell(nT+1,1); xms=cell(nT+1,1);
109     n=1;
110     tms{n} = reshape(relax_t,[],1);
111     xms{n} = relax_IC;
112
113     if saveSvf
114         svf.t = cell(nT+1,1);
115         svf.dx = cell(nT+1,1);
116     end
117 end

```

The idea of **PIG()** is to use the output from the microsolver to approximate an unknown function **ff(t,x)**, that describes the slow dynamics. This approximation is then used in the user-defined ‘coarse solver’ **csolve()**. The approximation is described in

```

128 function [dx]=genProjection(tt,xx)

```

Run a microsolver from the given initial conditions.

```

134 [t_tmp,x_micro_tmp] = solver(tt,reshape(xx,[],1),bT);

```

Compute the standard PI approximation of the slow vector field.

```

140 del = t_tmp(end)-t_tmp(end-1);
141 dx = (x_micro_tmp(end,:)-x_micro_tmp(end-1,:))/(del);

```

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

```

147 if saveMicro
148     n=n+1;
149     tms{n} = [reshape(t_tmp,[],1); nan];
150     xms{n} = [x_micro_tmp; nan(1,sIC)];
151     if saveSvf
152         svf.t{n-1} = tt;
153         svf.dx{n-1} = dx;
154     end
155 end

```

End `genProjection()`.

161 `end`

Define the approximate slow vector field according to PI.

169 `ff=@(t,x) genProjection(t,x);`

Do Projective Integration of `ff()` with the user-specified solver.

177 `[t,x]=feval(csolve,ff,tspan,relax_IC(end,:));`

Write over `x(1,:)` and `t(1)`, which the user expect to be `IC` and `tspan(1)` respectively, with the given initial conditions.

185 `x(1,:)=IC';`

186 `t(1)=tspan(1);`

Output the macroscale steps:

193

For each additional requested output, concatenate all the cells of time and state data into two arrays. Then, return the two arrays in a cell.

201 `if saveMicro`

202     `tms = cell2mat(tms);`

203     `xms = cell2mat(xms);`

204     `if saveSvf`

205         `svf.t = cell2mat(svf.t);`

206         `svf.dx = cell2mat(svf.dx);`

207     `end`

208 `end`

This concludes `PIG()`.

216 `end`

### 3.5 Example 2: PI using General macrosolvers

In this example the PI-General scheme is applied to a singularly perturbed ordinary differential equation. The aim is to allow a standard non-stiff numerical integrator, e.g. `ode45()`, to be applied to a stiff problem on a slow, long time scale.

11 `clear`

Set time scale separation and model.

18 `epsilon = 1e-4;`

19 `f=@(t,x) [cos(x(1))*sin(x(2))*cos(t); (cos(x(1))-x(2))/epsilon];`

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

26 `solver = @(tIC, xIC,T) feval('ode45',f,[tIC tIC+T],xC);`

27 `bT=20*epsilon;`

Set initial conditions, and the time to be covered by the macrosolver. Set the macrosolver to be used as a standard, non-stiff integration scheme.

34 `IC = [1 3];`

35 `tspan=[0 40];`

36 `macro.tspan = tspan;`

37 `macro.solver = 'ode45';`

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

45 `tic`

46 `[t,x,tms,xms] = PIG(solver,bT,macro,IC);`

47 `tPI=toc;`

48 `fprintf(['PI took %f seconds, using ode45 as the '\n' ...`  
`'macrosolver.\n'],tPI)`

50 `tic`

51 `[t45,xode45] = ode45(f,[tspan(1) tspan(end)],IC);`

```

52 tODE45 = toc;
53
54 fprintf('Brute force ode45 took %f seconds.\n',tODE45)

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

63 figure; set(gcf,'PaperPosition',[0 0 14 10])
64 hold on
65 PIm=plot(tms,xms,'b.');
66 PI=plot(t,x,'bo');
67 ODE45=plot(t45,xode45,'r-','LineWidth',2);
68 legend([PI(1),ODE45(1),PIm(1)],'PI Solution',...
69      'Standard Solution','PI microsolver')
70 xlabel('Time')
71 ylabel('State')
72 axis([0 40 0 3])
73
74 figure; set(gcf,'PaperPosition',[0 0 14 10])
75 hold on
76 PI2=plot(t,x,'bo');
77 ODE452=plot(t45,xode45,'r-','LineWidth',2);
78
79 legend([PI2(1),ODE452(1)],'PI Solution','Standard Solution')
80 xlabel('Time')
81 ylabel('State')

```

The output is plotted in Figure 5.

Notes:

- the problem may be made more, or less, stiff by changing the time scale parameter `epsilon`. `PIG()` will handle a stiffer problem with ease; but if the problem is insufficiently stiff, then the algorithm will produce nonsense. This problem is handled by `cdmc()`; see Section 3.7.
- The mildly stiff problem in Example 3.3 may be efficiently solved by a standard solver, e.g. `ode45()`. The stiff but low dimensional

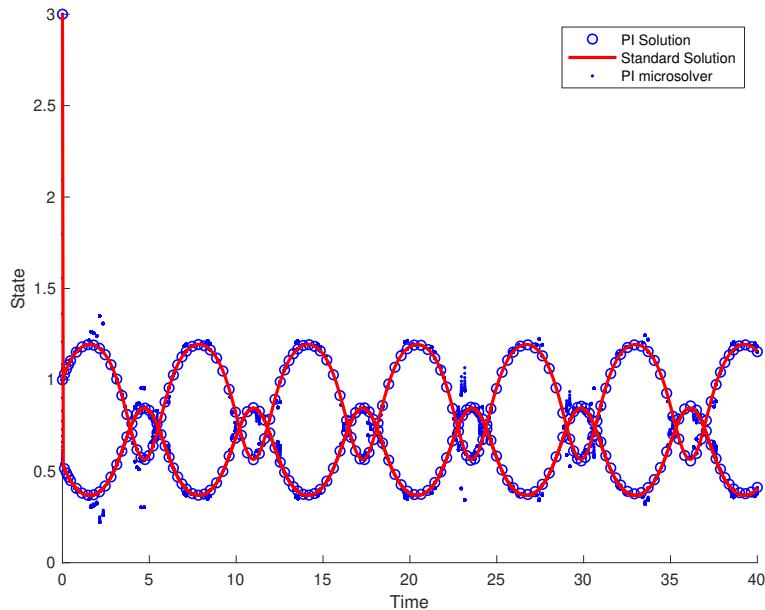


Figure 5: Accurate simulation of a stiff nonautonomous system by PIG(). The microsolver is called on-the-fly by the macrosolver (here `ode45`).

problem in this example can be solved efficiently by a standard stiff solver, e.g. `ode15s()`. The real advantage of the PI schemes is in high dimensional stiff problems, that cannot be efficiently solved by most standard methods.

## 3.6 Minor functions

### 3.6.1 `cdmc()`

`cdmc()` iteratively applies the microsolver and then projects backwards in time to the initial conditions. 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.

## Input

- **solver**, a black box microsolver suitable for PI. See any of **PIRK2()**, **PIRK4()**, **PIG()** for a description of **solver()**.
- **t**, an initial time
- **x**, an initial state
- **T**, a time period to apply **solver()** for

## Output

- **tout**, a vector of times. **tout(end)** will equal **t**.
- **xout**, an array of state estimates produced by **solver()**.

This function is a wrapper for the microsolver. For instance if the problem of interest is a dynamical system that is not too stiff, and which can be simulated by the solver **sol(t,x,T)**, one would define

```
cSol = @(t,x,T) cdmc(sol,t,x,T)|
```

and thereafter use **csol()** in place of **sol()** as the solver for any PI scheme. The original solver **sol()** would create large errors if used in a PI scheme, but the output of **cdmc()** will not.

33 `function [tout, xout] = cdmc(solver,t,x,T)`

Begin with a standard application of the microsolver.

39 `[tt,xx]=feval(solver,t,x,T);`

Project backwards to before the initial time, then simulate one burst forwards to obtain coordinates at **t**.

49 `del = (xx(end,:) - xx(end-1,:))/(tt(end) - tt(end-1));`

50 `b_prop = 0.2;`

51 `x = xx(end,:) + (1+b_prop)*(tt(1)-tt(end))*del;`

```
52 tr=2*tt(1)-tt(end);
53 [tout,xout]=feval(solver,tr,x',b_prop*T);
```

This concludes the function.

### 3.6.2 bbgen()

**bbgen()** is a simple function that takes a standard numerical method and produces a black box solver of the type required by the PI schemes.

```
12 function bb = bbgen(solver,f,dt)
```

#### Input

- **solver**, a standard numerical solver for ordinary differential equations
- **f**, a function  $f(t,x)$  taking time and state inputs
- **dt**, a time step suitable for simulation with **f**

**Output**  $bb = bb(t_{in}, x_{in}, T)$  a ‘black box’ microsolver that initialises at  $(t_{in}, x_{in})$  and simulates forward a duration  $T$ .

```
27 bb = @(t_in,x_in,T) feval(solver,f,...
28 linspace(t_in,t_in+T,1+ceil(T/dt)),x_in);
29 end
```

## 3.7 Explore: PI using constraint-defined manifold computing

In this example the PI-General scheme is applied to a singularly perturbed ordinary differential equation in which the time scale separation is not too strong. The resulting simulation is not accurate. In parallel, we run the same scheme but with **cdmc()** used as a wrapper for the microsolver. This second implementation successfully replicates the true dynamics.

10 clear

Set a weak time scale separation and model.

17 epsilon = 1e-2;

18 f=@(t,x) [cos(x(1))\*sin(x(2))\*cos(t); (cos(x(1))-x(2))/epsilon];

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

25 naiveSol = @(tIC, xIC,T) feval('ode45',f,[tIC tIC+T],xC);

26 bT=5\*epsilon;

Create a second struct in which the solver is the output of `cdmc()`.

32 cSol = @(t,x,T) cdmc(naiveSol,t,x,T);

Set initial conditions, and the time to be covered by the macrosolver. Set the macrosolver to be used as a standard, non-stiff integration scheme.

39 IC = [1 3];

40 tspan=0:0.5:40;

41 macro.tspan = tspan;

42 macro.solver = 'ode45';

Simulate using `PIG()` with each of the above microsolvers. Generate a trusted solution using standard numerical methods.

50 [nt,nx] = PIG(naiveSol,bT,macro,IC);

51 [ct,cx] = PIG(cSol,bT,macro,IC);

52 [t45,xode45] = ode45(f,[tspan(1) tspan(end)],IC);

Plot the output.

61 figure; set(gcf,'PaperPosition',[0 0 14 10])

62 hold on

63 nPI = plot(nt,nx,'bo');

64 PI=plot(ct,cx,'ko');

65 ODE45=plot(t45,xode45,'r-','LineWidth',2);

66

67 legend([nPI(1),PI(1),ODE45(1)],'Naive PIG Solution',...)

```

68      'PIG using cdmc', 'Accurate Solution')
69 xlabel('Time')
70 ylabel('State')
71 axis([0 40 0 3])

```

The output is plotted in Figure 6. The source of the error in the standard **PIG()** scheme is the burst length **bT**, that is significant on the slow time scale. Set **bT** to **20\*epsilon** or **50\*epsilon**<sup>1</sup> to worsen the error in both schemes. This example reflects a general principle, that most PI schemes will incur a global error term which is proportional to the simulation time of the microsolver and independent of the order of the microsolver. The **PIRK()** schemes have been written to minimise, if not eliminate entirely, this error, but by design **PIG()** works with any user-defined macrosolver and cannot reduce this error. The function **cdmc()** reduces this error term by attempting to mimic the microsolver without advancing time.

### 3.8 PIRK4(): projective integration of fourth order accuracy

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

```

15 function [x, tms, xms, rm, svf] = PIRK4(solver, bT, tSpan, x0)

```

The inputs and outputs are standardised with **PIRK2()**.

#### Input

- **solver()**, a function that produces output from the user-specified code for microscale simulation.

```
[tOut, xOut] = solver(tStart, xStart, tSim)
```

- Inputs: **tStart**, the start time of a burst of simulation; **xStart**, the row  $n$ -vector of the starting state; **tSim**, the total time to simulate in the burst.

---

<sup>1</sup>this example is quite extreme: at  $bT=50*\epsilon$ , it would be computationally much cheaper to simulate the entire length of `tspan` using the microsolver alone.

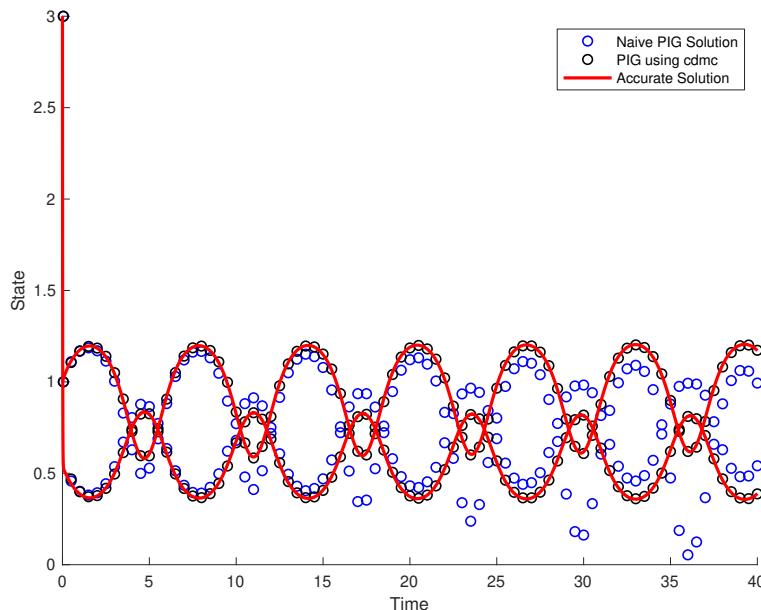


Figure 6: Accurate simulation of a weakly stiff nonautonomous system by PIG() using cdmc(), and an inaccurate solution using a naive application of PIG().

- Outputs: `tOut`, the column vector of solution times; and `xOut`, an array in which each *row* contains the system state at corresponding times.
- `bT`, a scalar, the minimum amount of time needed for simulation of the microsolver to relax the fast variables to the slow manifold.
- `tSpan` is an  $\ell$ -vector of times at which the user requests output, of which the first element is always the initial time. `PIRK4()` does not use adaptive time stepping; the macroscale time steps are (nearly) the steps between elements of `tSpan`.
- `x0` is an  $n$ -vector of initial values at the initial time `tSpan(1)`. Elements of `x0` may be `NaN`: they are included in the simulation and output, and

often represent boundaries in space fields.

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

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

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

- `tms`, optional, is an  $L$  dimensional column vector containing microscale times of burst simulations, each burst separated by `NaN`;
- `xms`, optional, is an  $L \times n$  array of the corresponding microscale states—this data is an accurate simulation of the state and may help visualise more details of the solution.
- `rm`, optional, a struct containing the ‘remaining’ applications of the microsolver 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 in general resemble the true dynamics.

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

- `svf.dx` is a  $4\ell \times n$  array containing the estimated slow vector field.

### 3.8.1 The projective integration code

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

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

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

```
119 nArgs=nargout();
120 saveMicro = (nArgs>1);
121 saveFullMicro = (nArgs>3);
122 saveSvf = (nArgs>4);
```

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

```
135 x0 = reshape(x0,1,[]);
136 [relax_t,relax_x0] = solver(tSpan(1),x0,bT);
```

Use the end point of the microsolver as the initial conditions.

```
144 tSpan(1) = tSpan(1)+bT;
145 x(1,:)=relax_x0(end,:);
```

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

```
155 if saveMicro
156     tms = cell(nT,1);
```

```

157     xms = cell(nT,1);
158     tms{1} = reshape(relax_t,[],1);
159     xms{1} = relax_x0;
160     if saveFullMicro
161         rm.t = cell(nT,1);
162         rm.x = cell(nT,1);
163         if saveSvf
164             svf.t = nan(4*nT-4,1);
165             svf.dx = nan(4*nT-4,length(x0));
166         end
167     end
168 end

```

### Loop over the macroscale time steps

```

176 for jT = 2:nT
177     T = tSpan(jT-1);

```

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

```

185     if 4*abs(bT)>=abs(tSpan(jT)-T) & bT*(tSpan(jT)-T)>0
186         [t1,xm1] = solver(T, x(jT-1,:), tSpan(jT)-T);
187         x(jT,:) = xm1(end,:);
188         t2=nan; xm2=nan(1,size(xm1,2));
189         t3=nan; t4=nan; xm3=xm2; xm4 = xm2; dx1=xm2; dx2=xm2;
190     else

```

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

```

201     [t1,xm1] = solver(T, x(jT-1,:), bT);
202     del = t1(end)-t1(end-1);

```

Check for round-off error.

```

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

```

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

```

221     Dt = tSpan(jT)-T-bT;
222     dx1 = (xm1(end,:)-xm1(end-1,:))/del;

```

Project along **dx1** to form an intermediate approximation of **x**; run another application of the microsolver and form a second estimate of the slow vector field.

```

232     xint = xm1(end,:)+ (Dt/2-bT)*dx1;
233     [t2,xm2] = solver(T+Dt/2, xint, bT);
234     del = t2(end)-t2(end-1);
235     dx2 = (xm2(end,:)-xm2(end-1,:))/del;

236
237     xint = xm1(end,:)+ (Dt/2-bT)*dx2;
238     [t3,xm3] = solver(T+Dt/2, xint, bT);
239     del = t3(end)-t3(end-1);
240     dx3 = (xm3(end,:)-xm3(end-1,:))/del;

241
242     xint = xm1(end,:)+ (Dt-bT)*dx3;
243     [t4,xm4] = solver(T+Dt, xint, bT);
244     del = t4(end)-t4(end-1);
245     dx4 = (xm4(end,:)-xm4(end-1,:))/del;

```

Check for round-off error.

```

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

```

254       **end**

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

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

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

270       **end**

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

280       **if** saveMicro  
 281            $tms\{jT\} = [\text{reshape}(t1, [], 1); \text{nan}]$ ;  
 282            $xms\{jT\} = [xm1; \text{nan}(1, \text{size}(xm1, 2))]$ ;

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

290       **if** saveFullMicro  
 291            $rm.t\{jT\} = [\text{reshape}(t2, [], 1); \text{nan}; \dots]$   
 292                    $\text{reshape}(t3, [], 1); \text{nan}; \dots]$   
 293                    $\text{reshape}(t4, [], 1); \text{nan}]$ ;  
 294            $rm.x\{jT\} = [xm2; \text{nan}(1, \text{size}(xm2, 2)); \dots]$   
 295                    $xm3; \text{nan}(1, \text{size}(xm2, 2)); \dots]$   
 296                    $xm4; \text{nan}(1, \text{size}(xm2, 2))]$ ;

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

305       **if** saveSvf  
 306            $svf.t(4*jT-7:4*jT-4) = [t1(end); t2(end); t3(end); t4(end)]$ ;  
 307            $svf.dx(4*jT-7:4*jT-4, :) = [dx1; dx2; dx3; dx4]$ ;  
 308       **end**  
 309       **end**  
 310       **end**

Terminate the main loop:

316 end

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

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

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

```
333 if saveMicro
334     tms = cell2mat(tms);
335     xms = cell2mat(xms);
336     if saveFullMicro
337         rm.t = cell2mat(rm.t);
338         rm.x = cell2mat(rm.x);
339     end
340 end
```

### 3.8.2 If no output specified, then plot simulation

```
348 if nArgs==0
349     figure, plot(tSpan,x,'o:')
350     title('Projective Simulation with PIRK4')
351 end
```

This concludes `PIRK4()`.

358 end

## 3.9 To do/discuss

- JM: did not change the introduction - seems to have been done? JB comments included?
- JM: need to discuss bibliography and style file handling. Do not understand current standard.

- JM: this file blends the standard code documentation with line-by-line code explanations and examples. Should have a preface/appendix/etc with just the standard code documentation
- JM: current code documentation (paragraph for Inputs and another for Outputs) goes counter to Matlab standard. Revert?
- AJR: inconsistency between description  $n$  and  $\ell$ , and the code's `N` and `n??` Proposed a partial answer. Also need to be clear what need to be row/column vectors.
- AJR: is there any advantage to `reshape(t2, [], 1)` over `t2(:)`? Answer appears to be nothing either way.
- AJR: can this code ‘integrate’ backwards in time using the forward time bursts? Answer: yes. But need to test its accuracy??
- AJR: remember, if used, cater for complex variable simulation by using real transpose `.'`.
- could implement Projective Integration by ‘arbitrary’ Runge–Kutta scheme; that is, by having the user input a particular Butcher table—surely only specialists would be interested
- can ‘reverse’ the order of projection and microsolver applications. The output at each user-requested coarse time would then be the end point of an application of the microsolver.
- Can maybe implement microsolvers that terminate a burst when the fast dynamics have settles using, for example, the ‘Events’ function handle in `ode23`.

## 4 Patch scheme for given microscale discrete space system

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The patch scheme applies to spatio-temporal systems where the spatial domain is larger than what can be computed in reasonable time. Then one may simulate 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 spatial discrete system is to be on a lattice such as obtained from finite difference approximation of a PDE. Usually continuous in time.

**Quick start** For an example, see Sections 4.1.1 and 4.7.1 for basic code that uses the provided functions to simulate Burgers' PDE and a nonlinear 'diffusion' PDE.

## 4.1 configPatches1(): configures spatial patches in 1D

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Makes the struct `patches` for use by the patch/gap-tooth time derivative function `patchSmooth1()`. Section 4.1.1 lists an example of its use.

```
17 function configPatches1(fun,Xlim,BCs,nPatch,ordCC,ratio,nSubP,nEdge)
18 global patches
```

**Input** If invoked with no input arguments, then executes an example of simulating Burgers' PDE—see Section 4.1.1 for the example code.

- `fun` is the name of the user function, `fun(t,u,x)`, that computes time derivatives (or time-steps) of quantities on the patches.
- `Xlim` give the macro-space domain of the computation: patches are equi-spaced over the interior of the interval `[Xlim(1), Xlim(2)]`.
- `BCs` somehow will define the macroscale boundary conditions. Currently, `BCs` is ignored and the system is assumed macro-periodic in the domain.

- **nPatch** is the number of equi-spaced spaced patches.
- **ordCC** is the ‘order’ of interpolation across empty space of the macroscale mid-patch values to the edge of the patches for inter-patch coupling: currently must be in  $\{-1, 0, \dots, 8\}$ .
- **ratio** (real) is the ratio of the half-width of a patch to the spacing of the patch mid-points: so  $\text{ratio} = \frac{1}{2}$  means the patches abut; and  $\text{ratio} = 1$  is overlapping patches as in holistic discretisation.
- **nSubP** is the number of equi-spaced microscale lattice points in each patch. Must be odd so that there is a central lattice point.
- **nEdge** is, for each patch, the number of edge values set by interpolation at the edge regions of each patch. May be omitted. The default is one (suitable for microscale lattices with only nearest neighbour interactions).

**Output** The *global* struct **patches** is created and set with the following components.

- **.fun** is the name of the user’s function **fun(u,t,x)** that computes the time derivatives (or steps) on the patchy lattice.
- **.ordCC** is the specified order of inter-patch coupling.
- **.alt** 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** are the **ordCC**-vector of weights for the inter-patch interpolation onto the right and left edges (respectively) with patch:macroscale ratio as specified.
- **.x** is **nSubP**  $\times$  **nPatch** array of the regular spatial locations  $x_{ij}$  of the microscale grid points in every patch.
- **.nEdge** is, for each patch, the number of edge values set by interpolation at the edge regions of each patch.

### 4.1.1 If no arguments, then execute an example

```
87 if nargin==0
```

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

1. configPatches1
2. ode15s integrator  $\leftrightarrow$  patchSmooth1  $\leftrightarrow$  user's burgersPDE
3. process results

Establish global patch data struct to interface with a function coding Burgers' PDE: to be solved on  $2\pi$ -periodic domain, with eight patches, spectral interpolation couples the patches, each patch of half-size ratio 0.2, and with seven points within each patch.

```
106 configPatches1(@BurgersPDE, [0 2*pi], nan, 8, 0, 0.2, 7);
```

Set an initial condition, and integrate in time using standard functions.

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

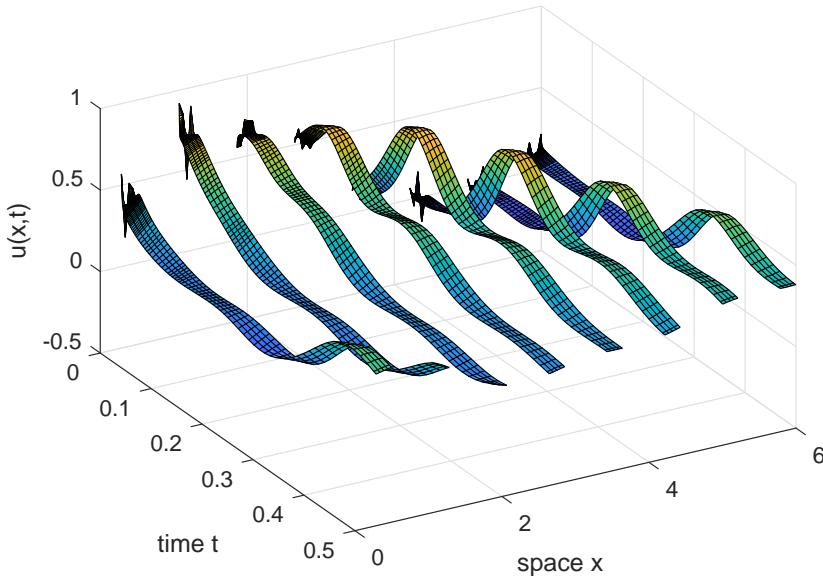
```
114 [ts,ucts]=ode15s(@patchSmooth1,[0 0.5],u0(:));
```

Plot the simulation using only the microscale values interior to the patches: set  $x$ -edges to `nan` to leave the gaps. [Figure 7](#) illustrates an example simulation in time generated by the patch scheme applied to Burgers' PDE.

```
124 figure(1),clf
125 patches.x([1 end],:)=nan;
126 surf(ts,patches.x(:,ucts'), view(60,40)
127 title('Example of Burgers PDE on patches in space')
128 xlabel('time t'), ylabel('space x'), zlabel('u(x,t)')
```

Upon finishing execution of the example, exit this function.

```
140 return
141 end%if no arguments
```

Figure 7: field  $u(x, t)$  of the patch scheme applied to Burgers' PDE.**Example of Burgers PDE on patches in space**

**Example of Burgers PDE inside patches** As a microscale discretisation of  $u_t = u_{xx} - 30uu_x$ , code  $\dot{u}_{ij} = \frac{1}{\delta x^2}(u_{i+1,j} - 2u_{i,j} + u_{i-1,j}) - 30u_{ij}\frac{1}{2\delta x}(u_{i+1,j} - u_{i-1,j})$ .

```

152 function ut=BurgersPDE(t,u,x)
153 dx=diff(x(1:2)); % micro-scale spacing
154 i=2:size(u,1)-1; % interior points in patches
155 ut=nan(size(u)); % preallocate storage
156 ut(i,:)=diff(u,2)/dx^2 ...
157 -30*u(i,:).*(u(i+1,:)-u(i-1,:))/(2*dx);
158 end

```

### 4.1.2 The code to make patches

Set one edge-value to compute by interpolation if not specified by the user.  
Store in the struct.

```
173 if nargin<8, nEdge=1; end
174 if nEdge>1, error('multi-edge-value interp not yet implemented'), end
175 if 2*nEdge+1>nSubP, error('too many edge values requested'), end
176 patches.nEdge=nEdge;
```

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

```
185 patches.fun=fun;
```

Second, store the order of interpolation that is to provide the values for the inter-patch coupling conditions. Spectral coupling is **ordCC** of 0 and  $-1$ .

```
194 if ~ismember(ordCC, [-1:8])
195     error('ordCC out of allowed range [-1:8]')
196 end
197
```

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

```
204 patches.alt=mod(ordCC,2);
205 ordCC=ordCC+patches.alt;
206 patches.ordCC=ordCC;
```

Check for staggered grid and periodic case.

```
212 if patches.alt && (mod(nPatch,2)==1)
213     error('Require an even number of patches for staggered grid')
214 end
```

Might as well precompute the weightings for the interpolation of field values for coupling. (Could sometime extend to coupling via derivative values.)

```
222 if patches.alt % eqn (7) in \cite{Cao2014a}
223     patches.Cwtsr=[1
```

```

224     ratio/2
225     (-1+ratio^2)/8
226     (-1+ratio^2)*ratio/48
227     (9-10*ratio^2+ratio^4)/384
228     (9-10*ratio^2+ratio^4)*ratio/3840
229     (-225+259*ratio^2-35*ratio^4+ratio^6)/46080
230     (-225+259*ratio^2-35*ratio^4+ratio^6)*ratio/645120 ];
231 else %
232     patches.Cwtsr=[ratio
233         ratio^2/2
234         (-1+ratio^2)*ratio/6
235         (-1+ratio^2)*ratio^2/24
236         (4-5*ratio^2+ratio^4)*ratio/120
237         (4-5*ratio^2+ratio^4)*ratio^2/720
238         (-36+49*ratio^2-14*ratio^4+ratio^6)*ratio/5040
239         (-36+49*ratio^2-14*ratio^4+ratio^6)*ratio^2/40320 ];
240 end
241 patches.Cwtsr=patches.Cwtsr(1:ordCC);
242 patches.Cwtsl=(-1).^(1:ordCC)'-patches.alt).*patches.Cwtsr;

```

Third, set the centre of the patches in a the macroscale grid of patches assuming periodic macroscale domain.

```

251
252 X=linspace(Xlim(1),Xlim(2),nPatch+1);
253 X=X(1:nPatch)+diff(X)/2;
254 DX=X(2)-X(1);
255

```

Construct the microscale in each patch, assuming Dirichlet patch edges, and a half-patch length of **ratio · DX**.

```

263 if mod(nSubP,2)==0, error('configPatches1: nSubP must be odd'), end
264 i0=(nSubP+1)/2;
265 dx=ratio*DX/(i0-1);
266
267 patches.x=bsxfun(@plus,dx*(-i0+1:i0-1)',X); % micro-grid

```

268

269 end% function

Fin.

## 4.2 patchCoreSmooth1(): interface to time integrators

### *Subsubsection contents*

Input	71
Output	72

To simulate in time with spatial patches we often need to interface a users time derivative function with time integration routines such as `ode15s` or `PIRK2`. This function provides an interface. Either the sub-patch structure is *smooth* so that the patch centre-values are sensible macroscale variables, or the user chooses to average over a *core* of values in the centre of each patch with these averages providing sensible macroscale variables (no core averaging corresponds to a core of size one). Patch edge values are determined by macroscale interpolation of the patch-centre values or core-averaged values. Communicate patch-design variables to this function using the previously established global struct `patches`.

```
28 function dudt=patchCoreSmooth1(t,u)
29 global patches
```

### Input

- `u` is a vector of length `nSubP · nPatch · nVars` where there are `nVars` field values at each of the points in the `nSubP × nPatch` grid.
- `t` is the current time to be passed to the user's time derivative function.
- `patches` a struct set by `configPatches1()` with the following information used here.

- `.fun` is the name of the user's function `fun(t,u,x)` that computes the time derivatives on the patchy lattice. The array `u` has size `nSubP × nPatch × nVars`. Time derivatives must be computed into the same sized array, but herein the patch edge values are overwritten by zeros.
- `.x` is `nSubP × nPatch` array of the spatial locations  $x_{ij}$  of the microscale grid points in every patch. Currently it *must* be an equi-spaced lattice on both macro- and micro-scales.

## Output

- `dudt` is `nSubP · nPatch · nVars` vector of time derivatives, but with patch edge values set to zero.

Reshape the fields `u` as a 2/3D-array, and sets the edge values from macroscale interpolation of centre-patch values. [Section 4.3](#) describes `patchEdgeInt1()`.

73   `u=patchCoreEdgeInt1(u);`

Ask the user function for the time derivatives computed in the array, overwrite its edge values with the dummy value of zero, then return to a to the user/integrator as column vector.

83   `dudt=patches.fun(t,u,patches.x);`  
 84   `dudt([1 end],:,:)=0;`  
 85   `dudt=reshape(dudt,[],1);`

Fin.

### 4.3 `patchEdgeInt1()`: sets edge values from interpolation over the macroscale

#### *Subsubsection contents*

<a href="#">Input</a>	73
<a href="#">Output</a>	73
<a href="#">Lagrange interpolation gives patch-edge values</a>	75

## Case of spectral interpolation . . . . . 76

Couples 1D patches across 1D space by computing their edge values from macroscale interpolation. Consequently a spatially discrete system could be integrated in time via the patch or gap-tooth scheme ([Roberts & Kevrekidis 2007](#)). Assumes that the sub-patch structure or core averages are *smooth* so are sensible macroscale variables, and patch edge values are determined by macroscale interpolation of the patch-centre values or patch cores. Communicate patch-design variables via the global struct `patches`.

```
22 function u=patchCoreEdgeInt1(u)
23 global patches
```

### Input

- `u` is a vector of length `nSubP · nPatch · nVars` where there are `nVars` field values at each of the points in the `nSubP × nPatch` grid.
- `patches` a struct set by `configPatches1()` which includes the following.
  - `.x` is `nSubP × nPatch` array of the spatial locations  $x_{ij}$  of the microscale grid points in every patch. Currently it *must* be an equi-spaced lattice on both macro- and micro-scales.
  - `.ordCC` is order of interpolation, currently in  $\{0, 2, 4, 6, 8\}$ .
  - `.alt` in  $\{0, 1\}$  is one for staggered grid (alternating) interpolation.
  - `.Cwtsr` and `.Cwtsl`

### Output

- `u` is `nSubP × nPatch × nVars` 2/3D array of the fields with edge values set by interpolation.

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

```

62 [nSubP,nPatch]=size(patches.x);
63 nVars=round(numel(u)/numel(patches.x));
64 %if numel(u) ~= nSubP*nPatch*nVars
65 % nSubP=nSubP; nPatch=nPatch; nVars=nVars; sizeu=size(u);
66 %end
67 u=reshape(u,nSubP,nPatch,nVars);

```

With Dirichlet patches, the half-length of a patch is  $h = dx(n_\mu - 1)/2$  (or  $-2$  for specified flux), and the ratio needed for interpolation is then  $r = h/\Delta X$ . Compute lattice sizes from inside the patches as the edge values may be NaNs, etc.

```

77 dx=patches.x(3,1)-patches.x(2,1);
78 DX=patches.x(2,2)-patches.x(2,1);
79

```

If the user has not defined the patch core, then we assume it to be a single point in the middle of the patch. For `patches.nCore`  $\neq 1$  the half width ratio is reduced, as described by [Bunder et al. \(2017\)](#).

```

88 %r=dx*(nSubP-1)/2/DX;
89 if isfield(patches,'nCore') == 0
90     patches.nCore=1;
91 end
92 r=dx*(nSubP-1)/2/DX*(nSubP - patches.nCore)/(nSubP - 1);

```

For the moment assume the physical domain is macroscale periodic so that the coupling formulas are simplest. Should eventually cater for periodic, odd-mid-gap, even-mid-gap, even-mid-patch, dirichlet, neumann, ?? These index vectors point to patches and their two immediate neighbours.

```
103 j=1:nPatch; jp=mod(j,nPatch)+1; jm=mod(j-2,nPatch)+1;
```

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

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

**Lagrange interpolation gives patch-edge values** So compute centred differences of the ensemble averaged patch core values for the macro-interpolation of all fields. Assumes the domain is macro-periodic.

```

121
122 if patches.ordCC>0 % then non-spectral interpolation
123
124 if patches.EnsAve
125   ucore=sum(mean(u((i0-c):(i0+c),j,:),3),1)';
126   dmu=zeros(patches.ordCC,nPatch);
127 else
128   ucore=reshape(sum(u((i0-c):(i0+c),j,:),1),nPatch,nVars);
129   dmu=zeros(patches.ordCC,nPatch,nVars);
130 end;
131 if patches.alt % use only odd numbered neighbours
132   dmu(1,:,:)=r*(ucore(jp,:)+ucore(jm,:))/2; % \mu
133   dmu(2,:,:)=r^2*(ucore(jp,:)-ucore(jm,:)); % \delta
134   jp=jp(jp); jm=jm(jm); % increase shifts to \pm2
135 else % standard
136   dmu(1,j,:)=r*(ucore(jp,:)-ucore(jm,:))/2; % \mu\delta
137   dmu(2,j,:)=r^2*(ucore(jp,:)-2*ucore(j,:)+ucore(jm,:))/2; % \delta\delta
138 end% if odd/even

```

Recursively take  $\delta^2$  of these to form higher order centred differences (could unroll a little to cater for two in parallel).

```

146 for k=1:(patches.ordCC/2-1)
147   dmu(2*k+1,:,:)=(r^2-k^2)*(dmu(2*k-1,jp,:)-2*dmu(2*k-1,j,:)+dmu(2*k,j));
148   dmu(2*k+2,:,:)=(r^2-k^2)*(dmu(2*k,jp,:)-2*dmu(2*k,j,:)+dmu(2*k,j));
149 end

```

Interpolate macro-values to be Dirichlet edge values for each patch ([Roberts & Kevrekidis 2007](#)), using weights computed in `configPatches1()`. Here interpolate to specified order.

```

157 if patches.EnsAve
158   u(nSubP,j,:)=repmat(ucore(j)'*(1-patches.alt) ...

```

```

159      +sum(dmu(:,:,1),[1,1,nVars]) ...
160      -sum(u((nSubP-patches.nCore+1):(nSubP-1),:,:),1);
161      u(1,j,:)=repmat(ucore(j)'*(1-patches.alt) ...
162      -sum(dmu(1:2:end,:),1)+sum(dmu(2:2:end,:),1),[1,1,nVars]) ...
163      -sum(u(2:patches.nCore,:,:),1);
164  else
165      u(nSubP,j,:)=ucore(j,:)*(1-patches.alt) ...
166      - reshape(sum(u((nSubP-patches.nCore+1):(nSubP-1),j,:),1),nPatches,
167      + reshape(sum(dmu(1:2:end,j,:),1) + sum(dmu(2:2:end,j,:),1),nPatches);
168      u(1,j,:)=ucore(j,:)*(1-patches.alt) ...
169      -reshape(sum(u(2:patches.nCore,j,:),1),nPatches,nVars) ...
170      + reshape(-sum(dmu(1:2:end,j,:),1) + sum(dmu(2:2:end,j,:),1),nPatches);
171 end;

```

**Case of spectral interpolation** Assumes the domain is macro-periodic. As the macroscale fields are  $N$ -periodic, the macroscale Fourier transform writes the centre-patch values as  $U_j = \sum_k C_k e^{ik2\pi j/N}$ . Then the edge-patch values  $U_{j\pm r} = \sum_k C_k e^{ik2\pi/N(j\pm r)} = \sum_k C'_k e^{ik2\pi j/N}$  where  $C'_k = C_k e^{ikr2\pi/N}$ . For `nPatch` patches we resolve ‘wavenumbers’  $|k| < \text{nPatch}/2$ , so set row vector `ks` =  $k2\pi/N$  for ‘wavenumbers’  $k = (0, 1, \dots, k_{\max}, -k_{\max}, \dots, -1)$  for odd  $N$ , and  $k = (0, 1, \dots, k_{\max}, \pm(k_{\max} + 1), -k_{\max}, \dots, -1)$  for even  $N$ .

```
188 else% spectral interpolation
```

Deal with staggered grid by doubling the number of fields and halving the number of patches (`configPatches1` tests there are an even number of patches). Then the patch-ratio is effectively halved. The patch edges are near the middle of the gaps and swapped.

```

198 if patches.alt % transform by doubling the number of fields
199 v=nan(size(u)); % currently to restore the shape of u
200 u=cat(3,u(:,1:2:nPatch,:),u(:,2:2:nPatch,:));
201 altShift=reshape(0.5*[ones(nVars,1);-ones(nVars,1)],1,1,[]);
202 iV=[nVars+1:2*nVars 1:nVars]; % scatter interp to alternate field
203 r=r/2; % ratio effectively halved
204 nPatch=nPatch/2; % halve the number of patches

```

```

205     nVars=nVars*2;    % double the number of fields
206     else % the values for standard spectral
207         altShift=0;
208         iV=1:nVars;
209     end

```

Now set wavenumbers.

```

215     kMax=floor((nPatch-1)/2);
216     ks=2*pi/nPatch*(mod((0:nPatch-1)+kMax,nPatch)-kMax);

```

Test for reality of the field values, and define a function accordingly.

```

223     if imag(u(i0,:,:))==0, uclean=@(u) real(u);
224     else                 uclean=@(u) u;
225     end

```

Compute the Fourier transform of the patch centre-values for all the fields. If there are an even number of points, then zero the zig-zag mode in the FT and add it in later as cosine.

```

234     Ck=fft(u(i0,:,:));
235     if mod(nPatch,2)==0
236         Czz=Ck(1,nPatch/2+1,:)/nPatch;
237         Ck(1,nPatch/2+1,:)=0;
238     end

```

The inverse Fourier transform gives the edge values via a shift a fraction  $r$  to the next macroscale grid point. Enforce reality when appropriate.

```

246     u(nSubP,:,:iV)=uclean(ifft(bsxfun(@times,Ck ...
247             ,exp(1i*bsxfun(@times,ks,altShift+r)))));
248     u( 1,:,:iV)=uclean(ifft(bsxfun(@times,Ck ...
249             ,exp(1i*bsxfun(@times,ks,altShift-r)))));

```

For an even number of patches, add in the cosine mode.

```

255     if mod(nPatch,2)==0
256         cosr=cos(pi*(altShift+r+(0:nPatch-1)));
257         u(nSubP,:,:iV)=u(nSubP,:,:iV)+uclean(bsxfun(@times,Czz,cosr));

```

```

258     cosr=cos(pi*(altShift-r+(0:nPatch-1)));
259     u( 1,:,iV)=u( 1,:,iV)+uclean(bsxfun(@times,Czz,cosr));
260 end

```

Restore staggered grid when appropriate. Is there a better way to do this??

```

267 if patches.alt
268   nVars=nVars/2;  nPatch=2*nPatch;
269   v(:,1:2:nPatch,:)=u(:, :,1:nVars);
270   v(:,2:2:nPatch,:)=u(:, :,nVars+1:2*nVars);
271   u=v;
272 end
273 end% if spectral

```

Fin, returning the 2/3D array of field values.

## 4.4 BurgersExample: simulate Burgers' PDE on patches

### *Subsection contents*

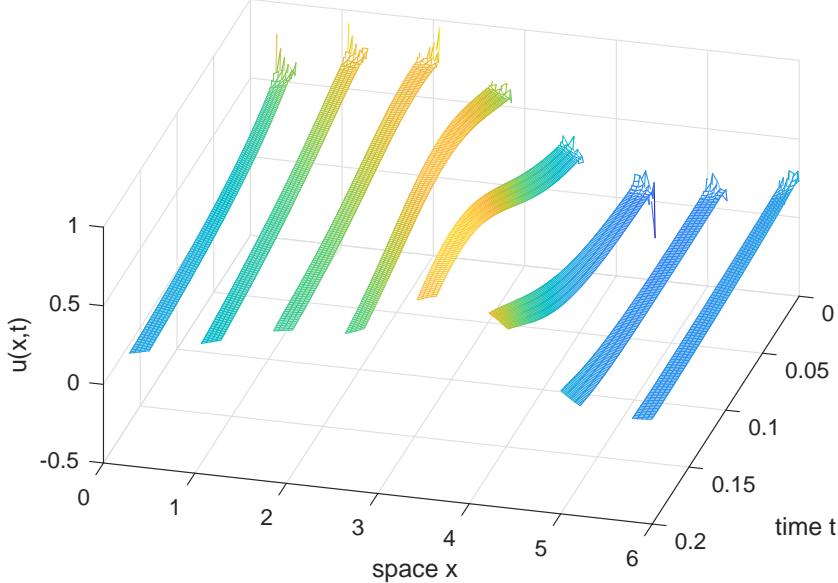
4.4.1	Script code to simulate a micro-scale space-time map .	79
4.4.2	burgersMap(): discretise the PDE microscale . . . . .	82
4.4.3	burgerBurst(): code a burst of the patch map . . . . .	83

Figure 7 shows an example simulation in time generated by the patch scheme function applied to Burgers' PDE. This code similarly applies the Equation-Free functions to a microscale space-time map (Figure 8), a map that happens to be derived as a micro-scale space-time discretisation of Burgers' PDE. Then this example applies projective integration to simulate further in time.

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

1. configPatches1
2. burgerBurst  $\leftrightarrow$  patchSmooth1  $\leftrightarrow$  burgersMap
3. process results

Figure 8: a short time simulation of the Burgers' map (Section 4.4.2) on patches in space. It requires many very small time steps only just visible in this mesh.



#### 4.4.1 Script code to simulate a micro-scale space-time map

Establish global data struct for the Burgers' map (Section 4.4.2) solved on  $2\pi$ -periodic domain, with eight patches, each patch of half-size ratio 0.2, with seven points within each patch, and say fourth order interpolation provides edge-values that couple the patches.

```

47 clear all
48 global patches
49 nPatch = 8
50 ratio = 0.2
51 nSubP = 7
52 interpOrd = 4
53 Len = 2*pi

```

54 configPatches1(@burgersMap, [0 Len], nan, nPatch, interpOrd, ratio, nSubP)

Set an initial condition, and simulate a burst of the micro-scale space-time map over a time 0.2 using the function `burgerBurst()` ([Section 4.4.3](#)).

62 u0 = 0.4\*(1+sin(patches.x))+0.1\*randn(size(patches.x));  
 63 [ts,us] = burgerBurst(0,u0,0.2);

Plot the simulation. Use only the microscale values interior to the patches via `nan` in the  $x$ -edges to leave gaps.

71 figure(1),clf  
 72 xs = patches.x; xs([1 end],:) = nan;  
 73 mesh(ts,xs(:,us'))  
 74 xlabel('time t'), ylabel('space x'), zlabel('u(x,t)')  
 75 view(105,45)  
 76 set(gcf,'paperposition',[0 0 14 10])  
 77 print('-depsc2','ps1BurgersMapU')

**Use projective integration** Around the micro-scale burst `burgerBurst()`, wrap the projective integration function `PIRK2()` of [Section 3.2](#). [Figure 9](#) shows the macroscale prediction of the patch centre values on macro-scale time-steps.

This second part of the script implements the following design.

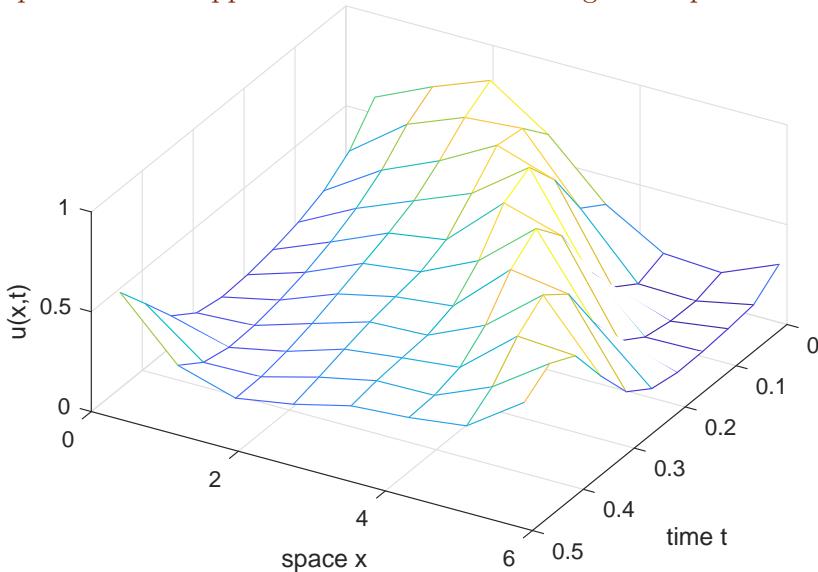
1. configPatches1 (done in first part)
2. PIRK2  $\leftrightarrow$  burgerBurst  $\leftrightarrow$  patchSmooth1  $\leftrightarrow$  burgersMap
3. process results

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

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

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

Figure 9: macro-scale space-time field  $u(x, t)$  in a basic projective integration of the patch scheme applied to the micro-scale Burgers' map.



```

118 ts = linspace(0,0.5,11);
119 bT = 3*(ratio*Len/nPatch/(nSubP/2-1))^2
120 addpath('..../ProjInt')
121 [us,tss,uss] = PIRK2(@burgerBurst,bT,ts,u0(:));

```

Plot the macroscale predictions of the mid-patch values to give the macroscale mesh of Figure 9.

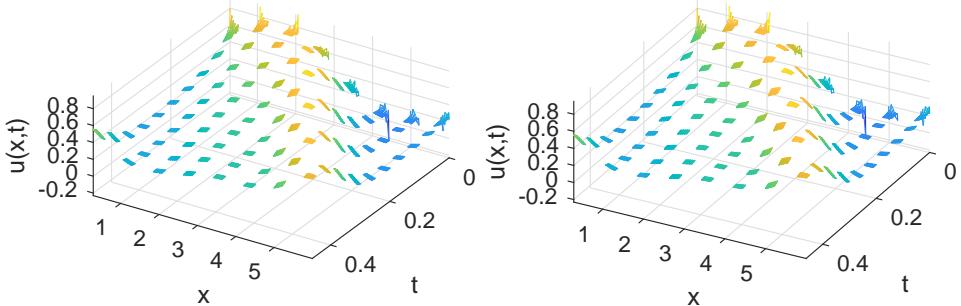
```

128 figure(2),clf
129 mid = (nSubP+1)/2;
130 mesh(ts,xs(mid,:),us(:,mid:nSubP:end)')
131 xlabel('time t'), ylabel('space x'), zlabel('u(x,t)')
132 view(120,50)
133 set(gcf,'paperposition',[0 0 14 10])
134 print('-depsc2','ps1BurgersU')

```

Then plot the microscale mesh of the microscale bursts shown in Figure 10

Figure 10: the field  $u(x, t)$  during each of the microscale bursts used in the projective integration. View this stereo pair cross-eyed.



(a stereo pair). The details of the fine microscale mesh are almost invisible.

```

148 figure(3),clf
149 for k = 1:2, subplot(2,2,k)
150   mesh(tss, xs(:, ),uss')
151   ylabel('x'), xlabel('t'), zlabel('u(x,t)')
152   axis tight, view(126-4*k,50)
153 end
154 set(gcf,'paperposition',[0 0 17 12])
155 print('-depsc2','ps1BurgersMicro')
```

#### 4.4.2 burgersMap(): discretise the PDE microscale

This function codes the microscale Euler integration map of the lattice differential equations inside the patches. Only the patch-interior values mapped (**patchSmooth1**) overrides the edge-values anyway).

```

172 function u = burgersMap(t,u,x)
173   dx = diff(x(2:3)); dt = dx^2/2;
174   i = 2:size(u,1)-1;
175   u(i,:) = u(i,:)+dt*( diff(u,2)/dx^2 ...
176     -20*u(i,:)*(u(i+1,:)-u(i-1,:))/(2*dx) );
177 end
```

#### 4.4.3 burgerBurst(): code a burst of the patch map

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

First find and set the number of micro-scale time-steps.

```
193 global patches
194 dt = diff(patches.x(2:3))^2/2;
195 ndt = ceil(bT/dt -0.2);
196 ts = ti+(0:ndt)'*dt;
```

Apply the microscale map over all time-steps in the burst, using `patchSmooth1` (Section 4.2) as the interface that provides the interpolated edge-values of each patch. Store the results in rows to be consistent with ODE and projective integrators.

```
206 us = nan(ndt+1,numel(ui));
207 us(1,:) = reshape(ui,1,[]);
208 for j = 1:ndt
209     ui = patchSmooth1(ts(j),ui);
210     us(j+1,:) = reshape(ui,1,[]);
211 end
```

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

```
218 ts(ndt+1) = ti+bT;
219 us(ndt+1,:) = us(ndt,:)
220     + diff(ts(ndt:ndt+1))/dt*diff(us(ndt:ndt+1,:));
221 end
```

Fin.

#### 4.5 HomogenisationCoreExample: simulate heterogeneous diffusion in 1D on patches

### Subsection contents

4.5.1	Script to simulate via stiff or projective integration . . . . .	85
4.5.2	<code>heteroDiff()</code> : heterogeneous diffusion . . . . .	93
4.5.3	<code>heteroBurst()</code> : a burst of heterogeneous diffusion . . . . .	93

Figure 11 and Figure 12 show example simulations in time generated by the patch scheme function applied to heterogeneous diffusion without and with an ensemble average, respectively. 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 minus the number of points in the core is an even multiple of the microscale periodicity (assuming the microscale periodicity is periodic on the macroscale domain).

We present two different methods of obtaining a macroscale solution. One method uses the given heterogeneous diffusion, which produces a solution which is rough at the microscale. The other method constructs an ensemble of heterogeneous diffusion and produces an ensemble average solution which is smooth at the microscale.

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

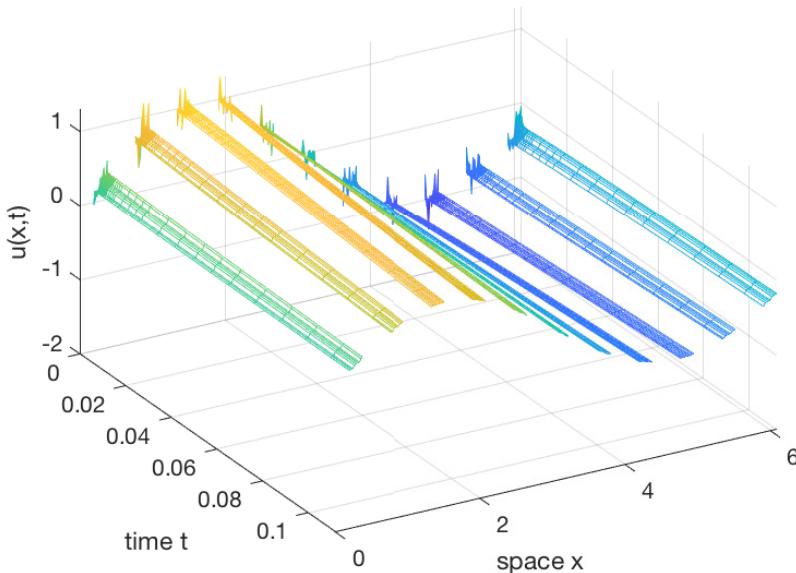
1. configPatches1
2.  $\text{ode15s} \leftrightarrow \text{patchSmooth1} \leftrightarrow \text{heteroDiff}$
3. process results

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

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

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

Figure 11: the diffusing field  $u(x, t)$  in the patch (gap-tooth) scheme applied to microscale heterogeneous diffusion with no ensemble average.



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

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

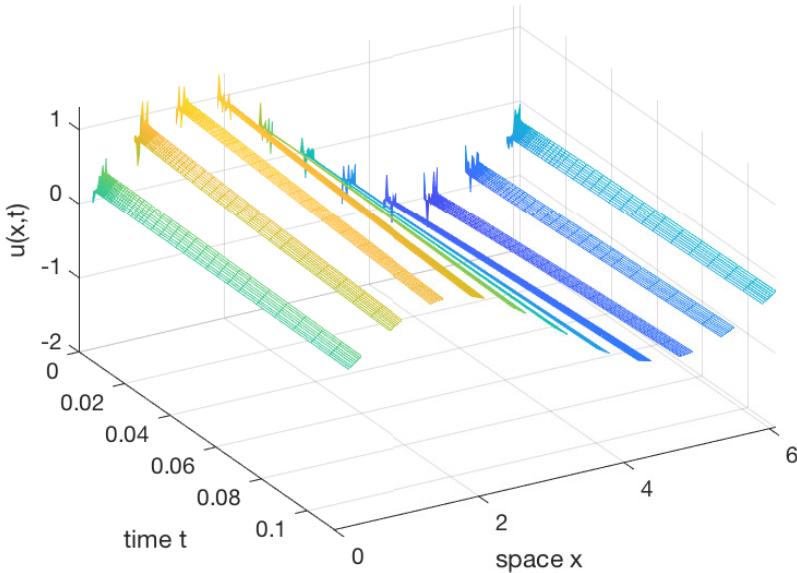
```

67 clear all
68 mPeriod = 4
69
70 rng('default'); rng(1);
71 sc=4;
72 cDiff = exp(sc*rand(mPeriod,1)); %2*abs(randn(mPeriod,1)); %exp(rand
73 cHomo = max(cDiff); %1/mean(1./cDiff);

```

Establish global data struct for heterogeneous diffusion solved on  $2\pi$ -periodic

Figure 12: the diffusing field  $u(x, t)$  in the patch (gap-tooth) scheme applied to microscale heterogeneous diffusion with an ensemble average.



domain, with eleven patches, each patch with half-size ratio 0.2, and the number of points in a patch minus the number of patches in a core equal to an even multiple of the microscale periodicity (which Bunder et al. (2017) showed is accurate). Quadratic (fourth-order) interpolation provides values for the inter-patch coupling conditions.

```

87 global patches
88 nPatch = 11
89 ratio = 0.2
90 nSubP = 11
91 Len = 2*pi;
92 configPatches1(@heteroDiff, [0 Len], nan, nPatch, 4, ratio, nSubP);

```

A user can add information to the global data struct **patches** in order to

communicate to the time derivative function. A  $(\text{nSubP}-1) \times \text{nPatch}$  matrix defines the diffusivity coefficients within each patch, but with ensemble averaging this must be increased to  $(\text{nSubP}-1) \times \text{nPatch} \times \text{nVars}$  (that is, when ensemble averaging  $\text{nVars}$  is the size of the ensemble; when we have no ensemble averaging  $\text{nVars}$  is the number of different field variables). The odd integer  $\text{patches.nCore} = 3$  defines the size of the patch core (this must be larger than zero and less than  $\text{nSubP}$ ), where a core of size zero indicates that the value in the centre of the patch is the macroscale. The introduction of a patch requires a redefinition of the half-patch ratio, as described by [Bunder et al. \(2017\)](#). We evaluate the patch coupling by interpolating the core and ensemble averaged field (although the latter only when  $\text{patches.Ens} = 1$ ).

```

116 patches.ordCC=6;
117 patches.cDiff = cDiff((mod(round(patches.x(1:(end-1),:)/(patches.x(2,
118 patches.nCore=3; %3
119 patches.ratio = ratio*(nSubP - patches.nCore)/(nSubP - 1);

```

The Boolean  $\text{patches.Ens}$  indicates whether or not we apply ensemble averaging of diffusivity configurations; if we do, then  $\text{nVars}$  becomes the size of the ensemble. When ensemble averaging we use the ensemble described by [Bunder et al. \(2017\)](#) which includes all reflected and translated configurations of  $\text{patches.cDiff}$ .

```

130 patches.EnsAve=0;
131 if patches.EnsAve
132   if mPeriod>2
133     nVars=2*mPeriod;
134   else
135     nVars=mPeriod;
136   end
137   patches.cDiff=repmat(patches.cDiff,[1,1,nVars]);
138   for sx=2:mPeriod
139     patches.cDiff(:,:,sx)=circshift(patches.cDiff(:,:,sx-1),[sx-1,0])
140   end;
141   if nVars>2
142     patches.cDiff(:,:, (mPeriod+1):end)=flipud(patches.cDiff(:,:,1:m

```

```
143     end;
144 end
```

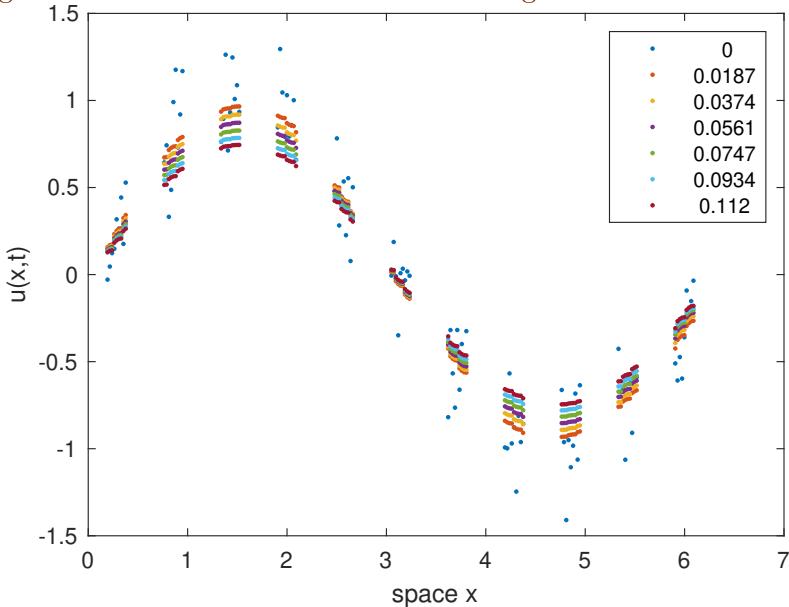
**Conventional integration in time** Set an initial condition, and here integrate forward in time using a standard method for stiff systems—because of the simplicity of linear problems this method works quite efficiently here. Integrate the interface `patchSmooth1` (Section 4.2) to the microscale differential equations.

```
157 u0 = sin(patches.x)+0.2*randn(nSubP,nPatch);
158 if patches.EnsAve
159     u0 = repmat(u0,[1,1,nVars]);
160 end
161 [ts,ucts] = ode15s(@patchCoreSmooth1, [0 2/cHomo], u0(:));
162 ucts=reshape(ucts,length(ts),length(patches.x(:)),[]);
```

Plot the simulation in Figure 11 (with no ensemble average) or Figure 12 (with an ensemble average). If we have calculated an ensemble of field solutions, we must first take the ensemble average.

```
171 if patches.EnsAve % calculate the ensemble average
172     uctsAve=mean(ucts,3);
173 else
174     uctsAve=ucts;
175 end
176 figure(1),clf
177 xs = patches.x;  xs([1 end],:) = nan;
178 mesh(ts,xs(:,uctsAve'), view(60,40)
179 xlabel('time t'), ylabel('space x'), zlabel('u(x,t)')
180
181 set(gcf,'PaperUnits','centimeters');
182 set(gcf,'PaperPosition',[0 0 14 10]);
183 if patches.EnsAve
184     print('-depsc2','ps1HomogenisationCoreCtsUEnsAve')
185 else
186     print('-depsc2','ps1HomogenisationCoreCtsU')
```

Figure 13: field  $u(x, t)$  shows basic projective integration of patches of heterogeneous diffusion with no ensemble average.



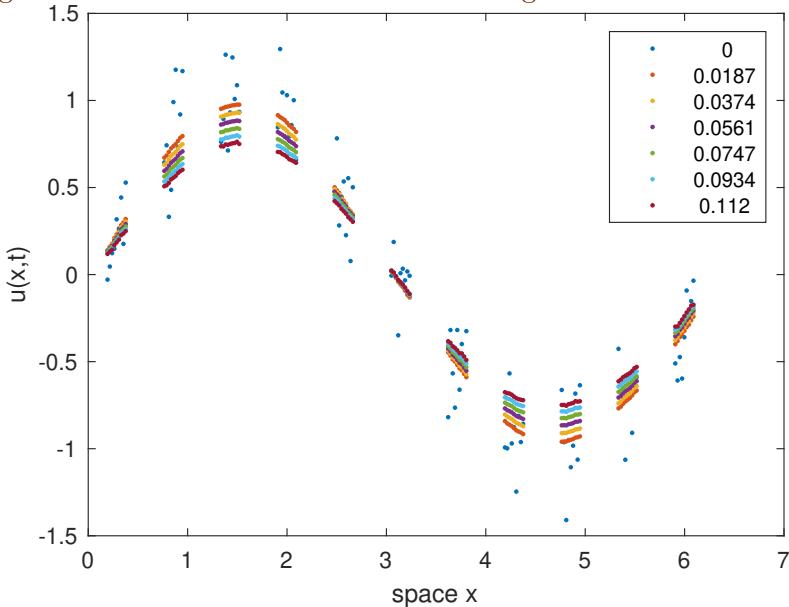
187    **end**

**Use projective integration in time** Now take `patchSmooth1`, the interface to the time derivatives, and wrap around it the projective integration `PIRK2` (Section 3.2), of bursts of simulation from `heteroBurst` (Section 4.5.3), as illustrated by Figure 13 and Figure 14.

This second part of the script implements the following design, where the micro-integrator could be, for example, `ode23` or `rk2int`.

1. configPatches1 (done in first part)
2. PIRK2  $\leftrightarrow$  heteroBurst  $\leftrightarrow$  micro-integrator  $\leftrightarrow$  patchSmooth1  $\leftrightarrow$  heteroDiff
3. process results

Figure 14: field  $u(x, t)$  shows basic projective integration of patches of heterogeneous diffusion with an ensemble average.



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

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

Set the desired macro- and micro-scale 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.

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

Plot the macroscale predictions to draw [Figure 13](#) or [Figure 14](#). If we have calculated an ensemble of field solutions, we must first take the ensemble average.

```

248 if patches.EnsAve % calculate the ensemble average
249   usAve=mean(reshape(us,size(us,1),length(xs(:)),nVars),3);
250   ussAve=mean(reshape(uss,length(tss),length(xs(:)),nVars),3);
251 else
252   usAve=us;
253   ussAve=uss;
254 end
255 figure(2),clf
256 plot(xs(:,usAve,'.')
257 ylabel('u(x,t)'), xlabel('space x')
258 legend(num2str(ts',3))
259 set(gcf,'PaperUnits','centimeters');
260 set(gcf,'PaperPosition',[0 0 14 10]);
261 if patches.EnsAve
262   print('-depsc2','ps1HomogenisationCoreUEnsAve')
263 else
264   print('-depsc2','ps1HomogenisationCoreU')
265 end

```

Also plot a surface detailing the microscale bursts as shown in [Figure 15](#) or [Figure 16](#).

```

285 figure(3),clf
286 for k = 1:2, subplot(1,2,k)
287   surf(tss,xs(:,ussAve,'EdgeColor','none')
288   ylabel('x'), xlabel('t'), zlabel('u(x,t)')
289   axis tight, view(126-4*k,45)
290 end
291 set(gcf,'PaperUnits','centimeters');
292 set(gcf,'PaperPosition',[0 0 14 6]);
293 if patches.EnsAve
294   print('-depsc2','ps1HomogenisationCoreMicroEnsAve')

```

Figure 15: stereo pair of the field  $u(x, t)$  during each of the microscale bursts used in the projective integration with no ensemble averaging.

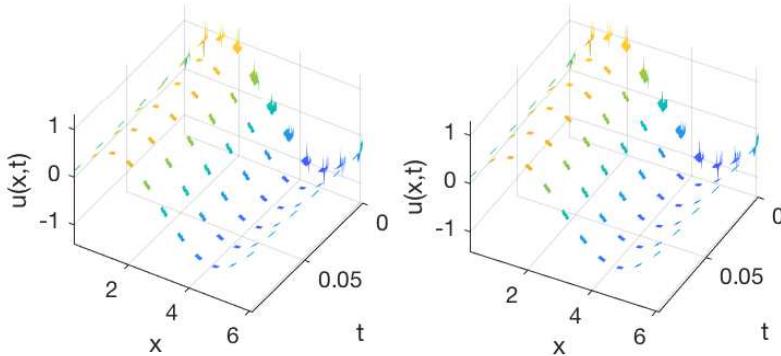
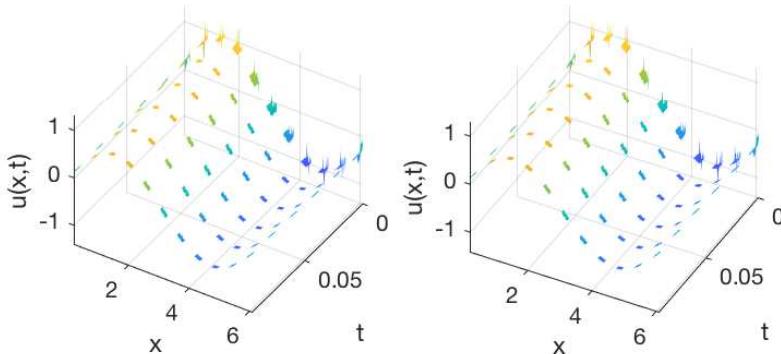


Figure 16: stereo pair of the field  $u(x, t)$  during each of the microscale bursts used in the projective integration with ensemble averaging.



```

295 else
296   print('-depsc2','ps1HomogenisationCoreMicro')
297 end

```

End of the script.

#### 4.5.2 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 **patchSmooth1**, Section 4.2), computes the time derivative (1) at each point in the interior of a patch, output in **ut**. The column vector (or possibly array) of diffusion coefficients  $c_i$  have previously been stored in struct **patches**.

```

315 function ut = heteroDiff(t,u,x)
316   global patches
317   dx = diff(x(2:3)); % space step
318   i = 2:size(u,1)-1; % interior points in a patch
319   ut = nan(size(u)); % preallocate output array
320   ut(i,:,:)=diff(patches.cDiff.*diff(u))/dx^2; %- abs(u(i,:,:)).*u
321 end

```

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

This code integrates in time the derivatives computed by **heteroDiff** from within the patch coupling of **patchSmooth1**. Try three possibilities:

- **ode23** generates ‘noise’ that is unsightly at best and may be ruinous;
- **ode15s** does not cater for the NaNs in some components of **u**;
- **rk2int** simple specified step integrator behaves consistently, and so appears best.

```

340 function [ts, ucts] = heteroBurst(ti, ui, bT)
341   switch 'rk2'
342     case '23',  [ts,ucts] = ode23 (@patchCoreSmooth1,[ti ti+bT],ui(:))

```

```

343 case '15s', [ts,ucts] = ode15s(@patchCoreSmooth1,[ti ti+bT],ui(:));
344 case 'rk2', ts = linspace(ti,ti+bT,200)';
345         ucts = rk2int(@patchCoreSmooth1,ts,ui(:));
346 end
347 end

```

Fin.

## 4.6 waterWaveExample: simulate a water wave PDE on patches

### *Subsection contents*

4.6.1	Script code to simulate wave systems . . . . .	96
4.6.2	simpleWavePDE(): simple wave PDE . . . . .	99
4.6.3	waterWavePDE(): water wave PDE . . . . .	100

[Figure 17](#) shows an example simulation in time generated by the patch scheme function applied to a simple wave PDE. The inter-patch coupling is realised by spectral interpolation to the patch edges of the mid-patch values.

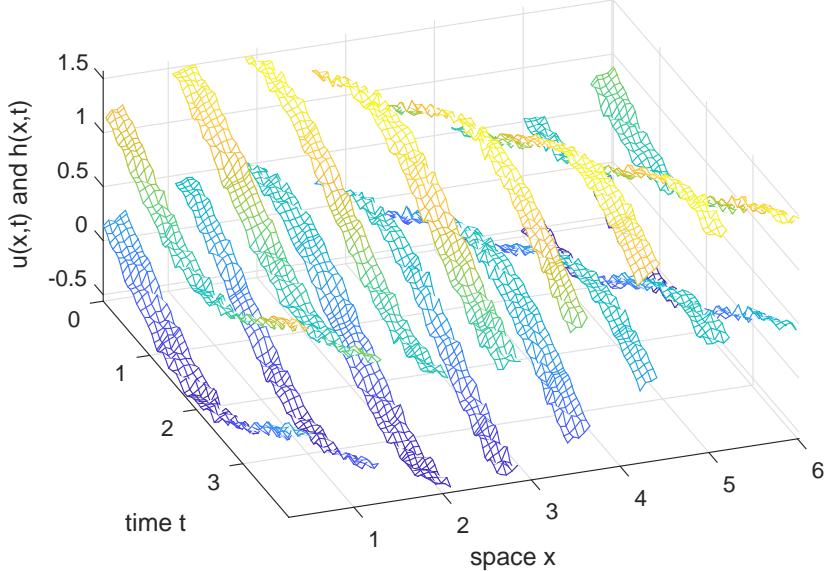
This approach, based upon the differential equations coded in [Section 4.6.2](#), may be adapted by a user to a wide variety of 1D wave and near-wave systems. For example, the differential equations of [Section 4.6.3](#) describes the nonlinear microscale simulator of the nonlinear shallow water wave PDE derived from the Smagorinski model of turbulent flow ([Cao & Roberts 2012, 2016a](#)).

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

$$\frac{\partial h}{\partial t} = -c_1 \frac{\partial u}{\partial x} + f_1[h, u] \quad \text{and} \quad \frac{\partial u}{\partial t} = -c_2 \frac{\partial h}{\partial x} + f_2[h, u], \quad (2)$$

where the brackets indicate that the nonlinear functions  $f_\ell$  may involve various spatial derivatives of the fields  $h(x, t)$  and  $u(x, t)$ . For example,

Figure 17: water depth  $h(x, t)$  (above) and velocity field  $u(x, t)$  (below) of the gap-tooth scheme applied to the simple wave PDE (2), linearised. The micro-scale random component to the initial condition has long lasting effects on the simulation—but the macroscale wave still propagates.



Section 4.6.3 encodes a nonlinear Smagorinski model of turbulent shallow water (Cao & Roberts 2012, 2016a, e.g.) along an inclined flat bed: let  $x$  measure position along the bed and in terms of fluid depth  $h(x, t)$  and depth-averaged lateral velocity  $u(x, t)$  the model PDEs are

$$\frac{\partial h}{\partial t} = -\frac{\partial(hu)}{\partial x}, \quad (3a)$$

$$\frac{\partial u}{\partial t} = 0.985 \left( \tan \theta - \frac{\partial h}{\partial x} \right) - 0.003 \frac{u|u|}{h} - 1.045u \frac{\partial u}{\partial x} + 0.26h|u| \frac{\partial^2 u}{\partial x^2}, \quad (3b)$$

where  $\tan \theta$  is the slope of the bed. Equation (3a) represents conservation of the fluid. The momentum PDE (3b) represents the effects of turbulent bed drag  $u|u|/h$ , self-advection  $u\partial u/\partial x$ , nonlinear turbulent dispersion  $h|u|\partial^2 u/\partial x^2$ , and gravitational hydrostatic forcing  $\tan \theta - \partial h/\partial x$ .

Figure 18: water depth  $h(x, t)$  (above) and velocity field  $u(x, t)$  (below) of the gap-tooth scheme applied to the Smagorinski shallow water wave PDEs (3). The micro-scale random initial component decays where the water speed is non-zero due to ‘turbulent’ dissipation.

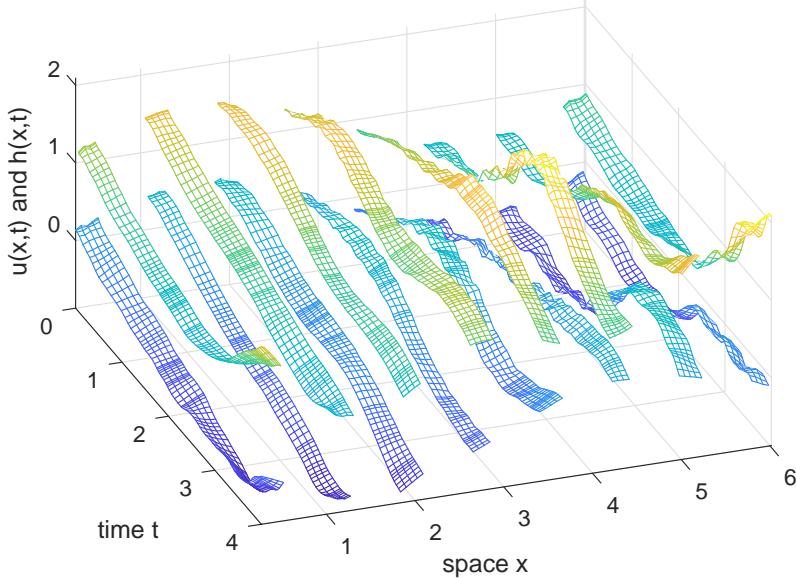


Figure 18 shows one simulation of this system—for the same initial condition as Figure 17.

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

#### 4.6.1 Script code to simulate wave systems

This script implements the following gap-tooth scheme (arrows indicate function recursion).

1. configPatches1, and add micro-information

2.  $\text{ode15s} \leftrightarrow \text{patchSmooth1} \leftrightarrow \text{simpleWavePDE}$
3. process results
4.  $\text{ode15s} \leftrightarrow \text{patchSmooth1} \leftrightarrow \text{waterWavePDE}$
5. process results

Establish the global data struct **patches** for the PDES (2) (linearised) solved on  $2\pi$ -periodic domain, with eight patches, each patch of half-size ratio 0.2, with eleven points within each patch, and third-order interpolation to provide edge-values for the inter-patch coupling conditions (higher order interpolation is smoother for smooth initial conditions).

```

71 clear all
72 global patches
73 nPatch = 8
74 ratio = 0.2
75 nSubP = 11 %of the form 4*n-1
76 Len = 2*pi;
77 configPatches1(@simpleWavePDE,[0 Len],nan,nPatch,-1,ratio,nSubP);

```

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

```

85 uPts = mod( bsxfun(@plus,(1:nSubP)',(1:nPatch)) ,2);
86 hPts = find(1-uPts);
87 uPts = find(uPts);
88 patches.hPts = hPts; patches.uPts = uPts;

```

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

```

96 U0 = nan(nSubP,nPatch);
97 U0(hPts) = 1+0.5*sin(patches.x(hPts));
98 U0(uPts) = 0+0.5*sin(patches.x(uPts));
99 U0 = U0+0.02*randn(nSubP,nPatch);

```

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

```
108 for k = 1:2
```

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

```
114 [ts,Ucts] = ode15s(@patchSmooth1,[0 4],U0(:));
115 ts = ts(1:5:end);
116 Ucts = Ucts(1:5:end,:);
```

Plot the simulation.

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

Print the output.

```
133 set(gcf,'paperposition',[0 0 14 10])
134 if k==1, print('-depsc2','ps1WaveCtsUH')
135 else print('-depsc2','ps1WaterWaveCtsUH')
136 end
```

For the second time through the loop, change to the Smagorinski turbulence model (3) of shallow water flow, keeping other parameters and the initial condition the same.

```
143 patches.fun = @waterWavePDE;
144 end
```

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

### 4.6.2 simpleWavePDE(): simple wave PDE

This function codes the staggered lattice equation inside the patches for the simple wave PDE system  $h_t = -u_x$  and  $u_t = -h_x$ . Here code for a staggered microscale grid of staggered macroscale patches: the array

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

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

```
237 function Ut = simpleWavePDE(t,U,x)
238   global patches
239   dx = diff(x(2:3));
240   Ut = nan(size(U)); ht = Ut;
```

Compute the PDE derivatives at interior points of the patches.

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

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

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

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

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

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

```
265 Ut(patches.hPts) = ht(patches.hPts);
266 end
```

### 4.6.3 waterWavePDE(): water wave PDE

This function codes the staggered lattice equation inside the patches for the nonlinear wave-like PDE system (3). Also, regularise the absolute value appearing the the PDEs via the one-line function `rabs()`.

```
278 function Ut = waterWavePDE(t,U,x)
279     global patches
280     rabs = @(u) sqrt(1e-4+u.^2);
```

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

```
286 dx = diff(x(2:3));
287 Ut = nan(size(U)); ht = Ut;
288 i = 2:size(U,1)-1;
```

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

```
294 ii = i(2:end-1);
295 V = Ut;
296 V(ii,:) = (U(ii+1,:)+U(ii-1,:))/2;
297 V(1:2,:) = 2*U(2:3,:)-V(3:4,:);
298 V(end-1:end,:) = 2*U(end-2:end-1,:)-V(end-3:end-2,:);
```

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

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

Correspondingly estimate the terms in the momentum PDE:  $u$ -values in  $\mathbf{U}_i$  and  $\mathbf{V}_{i\pm 1}$ ; and  $h$ -values in  $\mathbf{V}_i$  and  $\mathbf{U}_{i\pm 1}$ .

```
310 Ut(i,:) = -0.985*(U(i+1,:)-U(i-1,:))/(2*dx) ...
311     -0.003*U(i,:).*rabs(U(i,:)./V(i,:)) ...
312     -1.045*U(i,:).* (V(i+1,:)-V(i-1,:))/(2*dx) ...
313     +0.26*rabs(V(i,:).*U(i,:)).*(V(i+1,:)-2*U(i,:)+V(i-1,:))/dx^2/2;
```

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

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

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

```
326     Ut(patches.hPts) = ht(patches.hPts);
327 end
```

Fin.

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

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Makes the struct **patches** for use by the patch/gap-tooth time derivative function **patchSmooth2()**. Section 4.7.1 lists an example of its use.

```
17 function configPatches2(fun,Xlim,BCs,nPatch,ordCC,ratio,nSubP,nEdge)
18 global patches
```

**Input** If invoked with no input arguments, then executes an example of simulating a nonlinear diffusion PDE relevant to the lubrication flow of a thin layer of fluid—see [Section 4.7.1](#) for the example code.

- **fun** is the name of the user function, `fun(t,u,x,y)`, that computes time derivatives (or time-steps) of quantities on the patches.
- **Xlim** array/vector giving the macro-space domain of the computation: patches are equi-spaced over the interior of the rectangle  $[Xlim(1), Xlim(2)] \times [Xlim(3), Xlim(4)]$ : if of length two, then use the same interval in both directions, otherwise `Xlim(1:4)` give the interval in each direction.
- **BCs** somehow will define the macroscale boundary conditions. Currently, **BCs** is ignored and the system is assumed macro-periodic in the domain.
- **nPatch** determines the number of equi-spaced spaced patches: if scalar, then use the same number of patches in both directions, otherwise `nPatch(1:2)` give the number in each direction.
- **ordCC** is the ‘order’ of interpolation across empty space of the macroscale mid-patch values to the edge of the patches for inter-patch coupling: currently must be in {0}.
- **ratio** (real) is the ratio of the half-width of a patch to the spacing of the patch mid-points: so  $\text{ratio} = \frac{1}{2}$  means the patches abut; and  $\text{ratio} = 1$  would be overlapping patches as in holistic discretisation: if scalar, then use the same ratio in both directions, otherwise `ratio(1:2)` give the ratio in each direction.
- **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. Must be odd so that there is a central lattice point.
- **nEdge** is, for each patch, the number of edge values set by interpolation at the edge regions of each patch. May be omitted. The default is one (suitable for microscale lattices with only nearest neighbours. interactions).

**Output** The *global* struct **patches** is created and set with the following components.

- `.fun` is the name of the user's function `fun(u,t,x,y)` that computes the time derivatives (or steps) on the patchy lattice.
- `.ordCC` is the specified order of inter-patch coupling.
- `.alt` 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`-vector of weights for the inter-patch interpolation onto the right and left edges (respectively) with patch:macroscale ratio as specified.
- `.x` is `nSubP(1) × nPatch(1)` array of the regular spatial locations  $x_{ij}$  of the microscale grid points in every patch.
- `.y` is `nSubP(2) × nPatch(2)` array of the regular spatial locations  $y_{ij}$  of the microscale grid points in every patch.
- `.nEdge` is, for each patch, the number of edge values set by interpolation at the edge regions of each patch.

#### 4.7.1 If no arguments, then execute an example

```
100 if nargin==0
```

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

1. `configPatches2`
2. `ode15s` integrator  $\leftrightarrow$  `patchSmooth2`  $\leftrightarrow$  user's `nonDiffPDE`
3. process results

Establish global patch data struct to interface with a function coding a nonlinear ‘diffusion’ PDE: to be solved on  $6 \times 4$ -periodic domain, with  $9 \times 7$

patches, spectral interpolation couples the patches, each patch of half-size ratio 0.25, and with  $5 \times 5$  points within each patch.

```
120 nSubP = 5;
121 configPatches2(@nonDiffPDE, [-3 3 -2 2], nan, [9 7], 0, 0.25, nSubP);
```

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

```
128 x=reshape(patches.x,nSubP,1,[],1);
129 y=reshape(patches.y,1,nSubP,1,[]);
130 u0=exp(-x.^2-y.^2);
131 u0=u0.* (0.9+0.1*rand(size(u0)));
```

Initiate a plot of the simulation using only the microscale values interior to the patches: set  $x$  and  $y$ -edges to `nan` to leave the gaps. Start by showing the initial conditions of [Figure 19](#) while the simulation computes.

```
141 figure(1), clf
142 x=patches.x; y=patches.y;
143 x([1 end],:)=nan; y([1 end],:)=nan;
144 u = reshape(permute(u0,[1 3 2 4]), [numel(x) numel(y)]);
145 hsurf = surf(x(:,y(:,u'));
146 axis([-3 3 -3 3 -0.001 1]), view(60,40)
147 title('Nonlinear diffusion PDE on patches: solving with initial cond')
148 xlabel('space x'), ylabel('space y'), zlabel('u(x,y)')
149 drawnow
```

Integrate in time using standard functions.

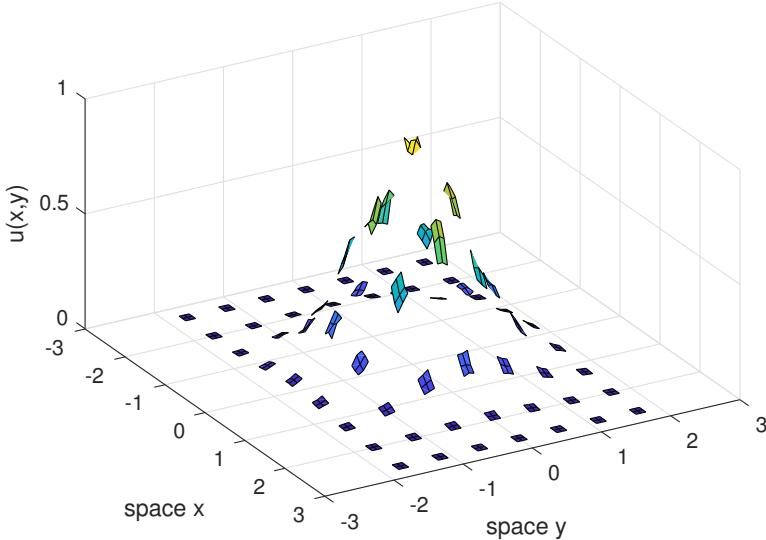
```
163 disp('Wait while we simulate h_t=(h^3)_xx+(h^3)_yy')
164 [ts,ucts]=ode15s(@patchSmooth2,[0 3],u0(:));
```

Animate the computed simulation to end with [Figure 20](#).

```
171 for i=1:length(ts)
172     u = patchEdgeInt2(ucts(i,:));
173     u = reshape(permute(u,[1 3 2 4]), [numel(x) numel(y)]);
174     hsurf.ZData = u';
175     title(['Nonlinear diffusion PDE on patches: time = ' num2str(ts(i))])
```

Figure 19: initial field  $u(x, y, t)$  at time  $t = 0$  of the patch scheme applied to a nonlinear ‘diffusion’ PDE: Figure 20 plots the computed field at time  $t = 3$ .

**Nonlinear diffusion PDE on patches: solving with initial condition**



```
176 pause(0.1)
```

```
177 end
```

Upon finishing execution of the example, exit this function.

```
192 return
```

```
193 end%if no arguments
```

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

```
204 function ut=nonDiffPDE(t,u,x,y)
```

```
205 dx=diff(x(1:2)); dy=diff(y(1:2)); % micro-scale spacing
```

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

```
207 ut=nan(size(u)); % preallocate storage
```

Figure 20: field  $u(x, y, t)$  at time  $t = 3$  of the patch scheme applied to a nonlinear ‘diffusion’ PDE with initial condition in [Figure 19](#).

```

208     ut(i,j,:,:)=diff(u(:,j,:,:).^3,2,1)/dx^2 ...
209                 +diff(u(i,:,:,:).^3,2,2)/dy^2;
210 end

```

#### 4.7.2 The code to make patches

Initially duplicate parameters as needed.

```

224 if numel(Xlim)==2, Xlim=repmat(Xlim,1,2); end
225 if numel(nPatch)==1, nPatch=repmat(nPatch,1,2); end
226 if numel(ratio)==1, ratio=repmat(ratio,1,2); end
227 if numel(nSubP)==1, nSubP=repmat(nSubP,1,2); end

```

Set one edge-value to compute by interpolation if not specified by the user.  
 Store in the struct.

```

235 if nargin<8, nEdge=1; end
236 if nEdge>1, error('multi-edge-value interp not yet implemented'), end
237 if 2*nEdge+1>nSubP, error('too many edge values requested'), end
238 patches.nEdge=nEdge;

```

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

```
247 patches.fun=fun;
```

Second, store the order of interpolation that is to provide the values for the inter-patch coupling conditions. Spectral coupling is **ordCC** of 0 and  $-1$ .

```

256 if ~ismember(ordCC,[0])
257     error('ordCC out of allowed range [0]')
258 end

```

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

```

265 patches.alt=mod(ordCC,2);
266 ordCC=ordCC+patches.alt;
267 patches.ordCC=ordCC;

```

Might as well precompute the weightings for the interpolation of field values for coupling. (Could sometime extend to coupling via derivative values.)

```

283 ratio=ratio(:)'; % force to be row vector
284 if patches.alt % eqn (7) in \cite{Cao2014a}
285     patches.Cwtsr=[1
286         ratio/2
287         (-1+ratio.^2)/8
288         (-1+ratio.^2).*ratio/48
289         (9-10*ratio.^2+ratio.^4)/384
290         (9-10*ratio.^2+ratio.^4).*ratio/3840
291         (-225+259*ratio.^2-35*ratio.^4+ratio.^6)/46080
292         (-225+259*ratio.^2-35*ratio.^4+ratio.^6).*ratio/645120 ];
293 else %
294     patches.Cwtsr=[ratio
295         ratio.^2/2

```

```

296     (-1+ratio.^2).*ratio/6
297     (-1+ratio.^2).*ratio.^2/24
298     (4-5*ratio.^2+ratio.^4).*ratio/120
299     (4-5*ratio.^2+ratio.^4).*ratio.^2/720
300     (-36+49*ratio.^2-14*ratio.^4+ratio.^6).*ratio/5040
301     (-36+49*ratio.^2-14*ratio.^4+ratio.^6).*ratio.^2/40320 ];
302 end
303 patches.Cwtsr=patches.Cwtsr(1:ordCC,:);
304 % should avoid this next implicit auto-replication
305 patches.Cwtsl=(-1).^(1:ordCC)'-patches.alt).*patches.Cwtsr;

```

Third, set the centre of the patches in a the macroscale grid of patches assuming periodic macroscale domain.

```

314 X=linspace(Xlim(1),Xlim(2),nPatch(1)+1);
315 X=X(1:nPatch(1))+diff(X)/2;
316 DX=X(2)-X(1);
317 Y=linspace(Xlim(3),Xlim(4),nPatch(2)+1);
318 Y=Y(1:nPatch(2))+diff(Y)/2;
319 DY=Y(2)-Y(1);

```

Construct the microscale in each patch, assuming Dirichlet patch edges, and a half-patch length of **ratio(1) · DX** and **ratio(2) · DY**.

```

327 nSubP=nSubP(:)'; % force to be row vector
328 if mod(nSubP,2)==[0 0], error('configPatches2: nSubP must be odd'),%
329 i0=(nSubP(1)+1)/2;
330 dx=ratio(1)*DX/(i0-1);
331 patches.x=bsxfun(@plus,dx*(-i0+1:i0-1)',X); % micro-grid
332 i0=(nSubP(2)+1)/2;
333 dy=ratio(2)*DY/(i0-1);
334 patches.y=bsxfun(@plus,dy*(-i0+1:i0-1)',Y); % micro-grid
335 end% function

```

Fin.

## 4.8 `patchSmooth2()`: interface to time integrators

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Output	110

To simulate in time with spatial patches we often need to interface a users time derivative function with time integration routines such as `ode15s` or `PIRK2`. This function provides an interface. It assumes that the sub-patch structure is *smooth* so that the patch centre-values are sensible macroscale variables, and patch edge values are determined by macroscale interpolation of the patch-centre values. Communicate patch-design variables to this function via the previously established global struct `patches`.

```
23 function dudt=patchSmooth2(t,u)
24 global patches
```

### **Input**

- `u` is a vector of length `prod(nSubP) · prod(nPatch) · nVars` where there are `nVars` 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,x,y)` that computes the time derivatives on the patchy lattice. The array `u` has size `nSubP(1) × nSubP(2) × nPatch(1) × nPatch(2) × nVars`. Time derivatives must be computed into the same sized array, but herein the patch edge values are overwritten by zeros.
  - `.x` is `nSubP(1) × nPatch(1)` array of the spatial locations  $x_{ij}$  of the microscale grid points in every patch. Currently it *must* be an equi-spaced lattice on both macro- and micro-scales.

- `.y` is similarly `nSubP(2) × nPatch(2)` array of the spatial locations  $y_{ij}$  of the microscale grid points in every patch. Currently it *must* be an equi-spaced lattice on both macro- and micro-scales.

## Output

- `dudt` is `prod(nSubP) · prod(nPatch) · nVars` vector of time derivatives, but with patch edge values set to zero.

Reshape the fields `u` as a 4/5D-array, and sets the edge values from macroscale interpolation of centre-patch values. [Section 4.9](#) describes `patchEdgeInt2()`.

76   `u=patchEdgeInt2(u);`

Ask the user function for the time derivatives computed in the array, overwrite its edge values with the dummy value of zero, then return to a to the user/integrator as column vector.

86   `dudt=patches.fun(t,u,patches.x,patches.y);`  
 87   `dudt([1 end],:,:,:,:)=0;`  
 88   `dudt(:,[1 end],:,:,:,:)=0;`  
 89   `dudt=reshape(dudt,[],1);`

Fin.

## 4.9 `patchEdgeInt2()`: sets 2D patch edge values from 2D macroscale interpolation

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<a href="#">Lagrange interpolation gives patch-edge values</a>	112
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Couples 2D patches across 2D space by computing their edge values via macroscale interpolation. Assumes that the sub-patch structure is *smooth*

so that the patch centre-values are sensible macroscale variables, and patch edge values are determined by macroscale interpolation of the patch-centre values. Communicate patch-design variables via the global struct `patches`.

```
21 function u=patchEdgeInt2(u)
22 global patches
```

## Input

- `u` is a vector of length  $\text{nx} \cdot \text{ny} \cdot \text{Nx} \cdot \text{Ny} \cdot \text{nVars}$  where there are `nVars` field values at each of the points in the  $\text{nx} \times \text{ny} \times \text{Nx} \times \text{Ny}$  grid on the  $\text{Nx} \times \text{Ny}$  array of patches.
- `patches` a struct set by `configPatches2()` which includes the following information.
  - `.x` is  $\text{nx} \times \text{Nx}$  array of the spatial locations  $x_{ij}$  of the microscale grid points in every patch. Currently it *must* be an equi-spaced lattice on both macro- and micro-scales.
  - `.y` is similarly  $\text{ny} \times \text{Ny}$  array of the spatial locations  $y_{ij}$  of the microscale grid points in every patch. Currently it *must* be an equi-spaced lattice on both macro- and micro-scales.
  - `.ordCC` is order of interpolation, currently only {0}.
  - `.Cwtsr` and `.Cwtsl`—not yet used

## Output

- `u` is  $\text{nx} \times \text{ny} \times \text{Nx} \times \text{Ny} \times \text{nVars}$  array of the fields with edge values set by interpolation.

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

```
67 [ny,Ny] = size(patches.y);
68 [nx,Nx] = size(patches.x);
69 nVars = round(numel(u)/numel(patches.x)/numel(patches.y));
```

```

70 if numel(u) ~= nx*ny*Nx*Ny*nVars
71   nSubP=[nx ny], nPatch=[Nx Ny], nVars=nVars, sizeu=size(u)
72 end
73 u = reshape(u,[nx ny Nx Ny nVars]);

```

With Dirichlet patches, the half-length of a patch is  $h = dx(n_\mu - 1)/2$  (or  $-2$  for specified flux), and the ratio needed for interpolation is then  $r = h/\Delta X$ . Compute lattice sizes from inside the patches as the edge values may be NaNs, etc.

```

83 dx = patches.x(3,1)-patches.x(2,1);
84 DX = patches.x(2,2)-patches.x(2,1);
85 rx = dx*(nx-1)/2/DX;
86 dy = patches.y(3,1)-patches.y(2,1);
87 DY = patches.y(2,2)-patches.y(2,1);
88 ry = dy*(ny-1)/2/DY;

```

For the moment assume the physical domain is macroscale periodic so that the coupling formulas are simplest. Should eventually cater for periodic, odd-mid-gap, even-mid-gap, even-mid-patch, dirichlet, neumann, ?? These index vectors point to patches and their two immediate neighbours.

```

99 %i=1:Nx; ip=mod(i,Nx)+1; im=mod(j-2,Nx)+1;
100 %j=1:Ny; jp=mod(j,Ny)+1; jm=mod(j-2,Ny)+1;

```

The centre of each patch (as **nx** and **ny** are odd) is at

```

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

```

**Lagrange interpolation gives patch-edge values** So compute centred differences of the mid-patch values for the macro-interpolation, of all fields. Assumes the domain is macro-periodic.

```

118 if patches.ordCC>0 % then non-spectral interpolation
119 error('non-spectral interpolation not yet implemented')
120 dmu=nan(patches.ordCC,nPatch,nVars);
121 % if patches.alt % use only odd numbered neighbours

```

```

122 % dmu(1,:,:)=(u(i0,jp,:)+u(i0,jm,:))/2; % \mu
123 % dmu(2,:,:)= u(i0,jp,:)-u(i0,jm,:); % \delta
124 % jp=jp(jp); jm=jm(jm); % increase shifts to \pm 2
125 % else % standard
126 dmu(1,:,:)=(u(i0,jp,:)-u(i0,jm,:))/2; % \mu\delta
127 dmu(2,:,:)=(u(i0,jp,:)-2*u(i0,j,:)+u(i0,jm,:)); % \delta^2
128 % end% if odd/even

```

Recursively take  $\delta^2$  of these to form higher order centred differences (could unroll a little to cater for two in parallel).

```

136 for k=3:patches.ordCC
137 dmu(k,:,:)=dmu(k-2,jp,:)-2*dmu(k-2,j,:)+dmu(k-2,jm,:);
138 end

```

Interpolate macro-values to be Dirichlet edge values for each patch ([Roberts & Kevrekidis 2007](#)), using weights computed in [`configPatches2\(\)`](#). Here interpolate to specified order.

```

146 u(nSubP,j,:)=u(i0,j,:)*(1-patches.alt) ...
147 +sum(bsxfun(@times,patches.Cwtsr,dmu));
148 u( 1,j,:)=u(i0,j,:)*(1-patches.alt) ...
149 +sum(bsxfun(@times,patches.Cwtsl,dmu));

```

**Case of spectral interpolation** Assumes the domain is macro-periodic. We interpolate in terms of the patch index  $j$ , say, not directly in space. As the macroscale fields are  $N$ -periodic in the patch index  $j$ , the macroscale Fourier transform writes the centre-patch values as  $U_j = \sum_k C_k e^{ik2\pi j/N}$ . Then the edge-patch values  $U_{j\pm r} = \sum_k C_k e^{ik2\pi/N(j\pm r)} = \sum_k C'_k e^{ik2\pi j/N}$  where  $C'_k = C_k e^{ikr2\pi/N}$ . For  $N$  patches we resolve ‘wavenumbers’  $|k| < N/2$ , so set row vector  $\mathbf{ks} = k2\pi/N$  for ‘wavenumbers’  $k = (0, 1, \dots, k_{\max}, -k_{\max}, \dots, -1)$  for odd  $N$ , and  $k = (0, 1, \dots, k_{\max}, \pm(k_{\max} + 1) - k_{\max}, \dots, -1)$  for even  $N$ .

```

170 else% spectral interpolation

```

Deal with staggered grid by doubling the number of fields and halving the number of patches ([`configPatches2`](#) tests there are an even number of

patches). Then the patch-ratio is effectively halved. The patch edges are near the middle of the gaps and swapped.

```

180 % if patches.alt % transform by doubling the number of fields
181 % error('staggered grid not yet implemented')
182 % v=nan(size(u)); % currently to restore the shape of u
183 % u=cat(3,u(:,1:2:nPatch,:),u(:,2:2:nPatch,:));
184 % altShift=reshape(0.5*[ones(nVars,1);-ones(nVars,1)],1,1,[]);
185 % iV=[nVars+1:2*nVars 1:nVars]; % scatter interp to alternate fie
186 % r=r/2; % ratio effectively halved
187 % nPatch=nPatch/2; % halve the number of patches
188 % nVars=nVars*2; % double the number of fields
189 % else % the values for standard spectral
190 % altShift = 0;
191 % iV = 1:nVars;
192 % end

```

Now set wavenumbers in the two directions. In the case of even  $N$  these compute the + -case for the highest wavenumber zig-zag mode,  $k = (0, 1, \dots, k_{\max}, +(k_{\max} + 1) - k_{\max}, \dots, -1)$ .

```

201 kMax = floor((Nx-1)/2);
202 krx = rx*2*pi/Nx*(mod((0:Nx-1)+kMax,Nx)-kMax);
203 kMay = floor((Ny-1)/2);
204 kry = ry*2*pi/Ny*(mod((0:Ny-1)+kMay,Ny)-kMay);

```

Test for reality of the field values, and define a function accordingly.

```

211 if imag(u(i0,j0,:,:,:))==0, uclean = @(u) real(u);
212 else uclean = @(u) u; end

```

Compute the Fourier transform of the patch centre-values for all the fields. If there are an even number of points, then zero the zig-zag mode in the FT and add it in later as cosine.

```

221 Ck = fft2(squeeze(u(i0,j0,:,:,:)));

```

The inverse Fourier transform gives the edge values via a shift a fraction  $rx/ry$  to the next macroscale grid point. Initially preallocate storage for all the

IFFTs that we need to cater for the zig-zag modes when there are an even number of patches in the directions.

```
232 nFTx = 2-mod(Nx,2);
233 nFTy = 2-mod(Ny,2);
234 unj = nan(1,ny,Nx,Ny,nVars,nFTx*nFTy);
235 u1j = nan(1,ny,Nx,Ny,nVars,nFTx*nFTy);
236 uin = nan(nx,1,Nx,Ny,nVars,nFTx*nFTy);
237 ui1 = nan(nx,1,Nx,Ny,nVars,nFTx*nFTy);
```

Loop over the required IFFTs.

```
243 iFT = 0;
244 for iFTx = 1:nFTx
245 for iFTy = 1:nFTy
246 iFT = iFT+1;
```

First interpolate onto  $x$ -limits of the patches. (It may be more efficient to product exponentials of vectors, instead of exponential of array—only for  $N > 100$ . Can this be vectorised further??)

```
255 for jj = 1:ny
256 ks = (jj-j0)*2/(ny-1)*kry; % fraction of kry along the edge
257 unj(1,jj,:,:,:,iV,iFT) = ifft2( bsxfun(@times,Ck ...
258 ,exp(1i*bsxfun(@plus,altShift+krx',ks))))';
259 u1j(1,jj,:,:,:,iV,iFT) = ifft2( bsxfun(@times,Ck ...
260 ,exp(1i*bsxfun(@plus,altShift-krx',ks))))';
261 end
```

Second interpolate onto  $y$ -limits of the patches.

```
267 for i = 1:nx
268 ks = (i-i0)*2/(nx-1)*kry; % fraction of kry along the edge
269 uin(i,1,:,:,:,iV,iFT) = ifft2( bsxfun(@times,Ck ...
270 ,exp(1i*bsxfun(@plus,ks',altShift+kry))))';
271 ui1(i,1,:,:,:,iV,iFT) = ifft2( bsxfun(@times,Ck ...
272 ,exp(1i*bsxfun(@plus,ks',altShift-kry))))';
273 end
```

When either direction have even number of patches then swap the zig-zag wavenumber to the conjugate.

```
280 if nFTy==2, kry(Ny/2+1) = -kry(Ny/2+1); end
281 end% iFTy-loop
282 if nFTx==2, krx(Nx/2+1) = -krx(Nx/2+1); end
283 end% iFTx-loop
```

Put edge-values into the  $u$ -array, using `mean()` to treat a zig-zag mode as cosine. Enforce reality when appropriate via `uclean()`.

```
291 u(end,:,:,:,iV) = uclean( mean(unj,6) );
292 u( 1 ,:,:, :,iV) = uclean( mean(u1j,6) );
293 u(:,end,:,:,:,iV) = uclean( mean(uin,6) );
294 u(:, 1 ,:,:, :,iV) = uclean( mean(ui1,6) );
```

Restore staggered grid when appropriate. Is there a better way to do this??

```
301 %if patches.alt
302 % nVars=nVars/2; nPatch=2*nPatch;
303 % v(:,1:2:nPatch,:)=u(:,:,1:nVars);
304 % v(:,2:2:nPatch,:)=u(:,:,nVars+1:2*nVars);
305 % u=v;
306 %end
307 end% if spectral
308 end% function patchEdgeInt2
```

Fin, returning the 4/5D array of field values with interpolated edges.

## 4.10 wave2D: example of a wave on patches in 2D

### *Subsection contents*

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4.10.2 Execute a simulation . . . . .	118
4.10.3 Example of simple wave PDE inside patches . . . . .	121

For  $u(x, y, t)$ , test and simulate the simple wave PDE in 2D space:

$$\frac{\partial^2 u}{\partial t^2} = \nabla^2 u.$$

This script shows one way to get started: a user's script may have the following three steps (arrows indicate function recursion).

1. configPatches2
2. ode15s integrator  $\leftrightarrow$  patchSmooth2  $\leftrightarrow$  wavePDE
3. process results

Establish global patch data struct to interface with a function coding the wave PDE: to be solved on  $2\pi$ -periodic domain, with  $9 \times 9$  patches, spectral interpolation couples the patches, each patch of half-size ratio 0.25, and with  $5 \times 5$  points within each patch.

```
33 clear all, close all
34 global patches
35 nSubP = 5;
36 nPatch = 9;
37 configPatches2(@wavePDE, [-pi pi], nan, nPatch, 0, 0.1, nSubP);
```

#### 4.10.1 Check on the linear stability of the wave PDE

Set a zero equilibrium as basis. Then find the patch-interior points as the only ones to vary in order to construct the Jacobian.

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

Now construct the Jacobian. Since linear wave PDE, use large perturbations.

```
58 small=1;
59 jac=nan(length(i));
```

```

60 sizejac=size(jac)
61 for j=1:length(i)
62     uv=uv0(:);
63     uv(i(j))=uv(i(j))+small;
64     tmp=patchSmooth2(0,uv)/small;
65     jac(:,j)=tmp(i);
66 end

```

Now explore the eigenvalues a little: find the ten with the biggest real-part; if small enough, then the method may be good.

```

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

```

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

```

85 kwave=0:(nPatch-1)/2;
86 freq=sort(reshape(sqrt(kwave'.^2+kwave.^2),1,[]));
87 freq= freq(diff([-1 freq])>1e-9);
88 freqerr=[freq; min(abs(imag(evals)-freq))]

```

#### 4.10.2 Execute a simulation

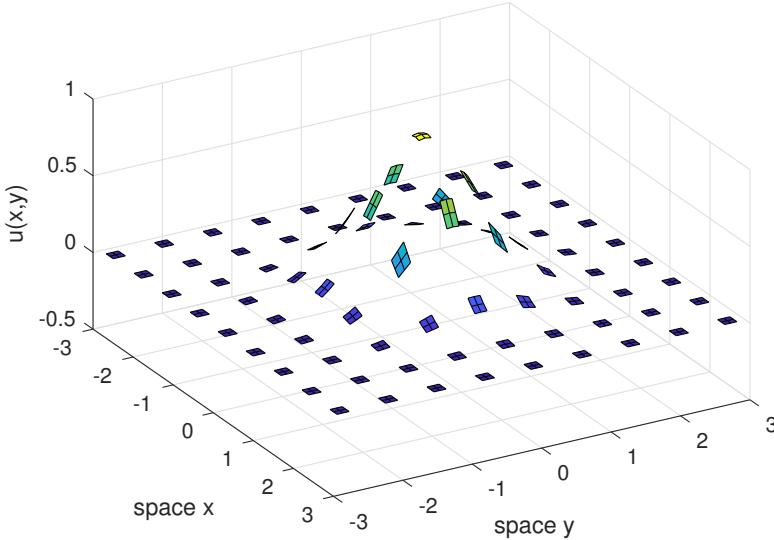
Set a Gaussian initial condition using auto-replication of the spatial grid: here **u0** and **v0** are in the form required for computation:  $n_x \times n_y \times N_x \times N_y$ .

```

101 x = reshape(patches.x,nSubP,1,[],1);
102 y = reshape(patches.y,1,nSubP,1,[]);
103 u0 = exp(-x.^2-y.^2);
104 v0 = zeros(size(u0));

```

Figure 21: initial field  $u(x, y, t)$  at time  $t = 0$  of the patch scheme applied to the simple wave PDE: [Figure 22](#) plots the computed field at time  $t = 6$ .



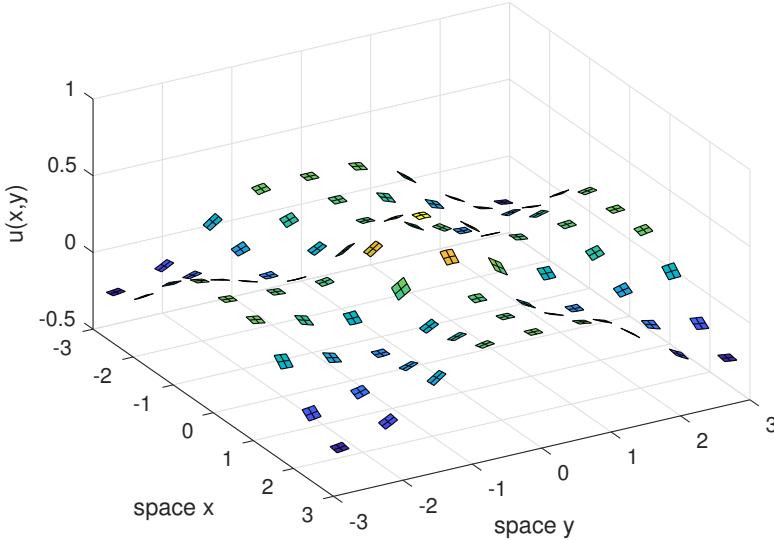
Initiate a plot of the simulation using only the microscale values interior to the patches: set  $x$  and  $y$ -edges to `nan` to leave the gaps. Start by showing the initial conditions of [Figure 19](#) while the simulation computes. To mesh/surf plot we need to ‘transpose’ to size  $n_x \times N_x \times n_y \times N_y$ , then reshape to size  $n_x \cdot N_x \times n_y \cdot N_y$ .

```

114 x=patches.x; y=patches.y;
115 x([1 end],:)=nan; y([1 end],:)=nan;
116 u = reshape(permute(u0,[1 3 2 4]), [numel(x) numel(y)]);
117 usurf = surf(x(:,y(:,u';
118 axis([-3 3 -3 3 -0.5 1]), view(60,40)
119 xlabel('space x'), ylabel('space y'), zlabel('u(x,y)')
120 drawnow
121 set(gcf,'paperposition',[0 0 14 10])
122 print('-depsc','wave2Dic.eps')
```

Integrate in time using standard functions.

Figure 22: field  $u(x, y, t)$  at time  $t = 6$  of the patch scheme applied to the simple wave PDE with initial condition in Figure 21.



```

136 disp('Wait while we simulate u_t=v, v_t=u_xx+u_yy')
137 [ts, uvs] = ode15s(@patchSmooth2, [0 1], [u0(:); v0(:)]);

```

Animate the computed simulation to end with Figure 22. Subsample to plot at most 200 times.

```

144 di = ceil(length(ts)/200);
145 for i = [1:di:length(ts)-1 length(ts)]
146   uv = patchEdgeInt2(uvs(i,:));
147   uv = reshape(permute(uv,[1 3 2 4 5]), [numel(x) numel(y) 2]);
148   usurf.ZData = uv(:,:,1)';
149   title(['wave PDE on patches: time = ' num2str(ts(i))])
150   pause(0.1)
151 end
152 title('')
153 set(gcf,'paperposition',[0 0 14 10])
154 print('-depsc',[ 'wave2Dt' num2str(ts(end)) '.eps'])

```

### 4.10.3 Example of simple wave PDE inside patches

As a microscale discretisation of  $u_{tt} = \nabla^2(u)$ , so code  $\dot{u}_{ijkl} = v_{ijkl}$  and  $\dot{v}_{ijkl} = \frac{1}{\delta x^2}(u_{i+1,j,k,l} - 2u_{i,j,k,l} + u_{i-1,j,k,l}) + \frac{1}{\delta y^2}(u_{i,j+1,k,l} - 2u_{i,j,k,l} + u_{i,j-1,k,l})$ .

```

174 function uvt = wavePDE(t,uv,x,y)
175   if ceil(t+1e-7)-t<2e-2, simTime=t, end %track progress
176   dx=diff(x(1:2)); dy=diff(y(1:2)); % micro-scale spacing
177   i=2:size(uv,1)-1; j=2:size(uv,2)-1; % interior patch-points
178   uvt = nan(size(uv)); % preallocate storage
179   uvt(i,j,:,:,:1) = uv(i,j,:,:,:2);
180   uvt(i,j,:,:,:2) = diff(uv(:,j,:,:,:1),2,1)/dx^2 ...
181                           +diff(uv(i,:,:,:,1),2,2)/dy^2;
182 end

```

## 4.11 To do

- Testing is so far only qualitative. Need to be quantitative.
- Multiple space dimensions.
- Heterogeneous microscale via averaging regions.
- Parallel processing versions.
- ??
- Adapt to maps in micro-time? Surely easy, just an example.

## 4.12 Miscellaneous tests

### 4.12.1 patchEdgeInt1test: test the spectral interpolation

*Subsubsection contents*

Test standard spectral interpolation . . . . .	122
Now test spectral interpolation on staggered grid . . .	123

Finish . . . . . 125

A script to test the spectral interpolation of function `patchEdgeInt1()`  
 Establish global data struct for the range of various cases.

```
13 clear all
14 global patches
15 nSubP=3
16 i0=(nSubP+1)/2; % centre-patch index
```

**Test standard spectral interpolation** Test over various numbers of patches, random domain lengths and random ratios.

```
24 for nPatch=5:10
25 nPatch=nPatch
26 Len=10*rand
27 ratio=0.5*rand
28 configPatches1(@sin,[0,Len],nan,nPatch,0,ratio,nSubP);
29 kMax=floor((nPatch-1)/2);
```

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

```
37 for k=-kMax:kMax
38 u0=exp(1i*k*patches.x*2*pi/Len);
39 ui=patchEdgeInt1(u0(:));
40 normError=norm(ui-u0);
41 if abs(normError)>5e-14
42 normError=normError
43 error(['failed single var interpolation k=' num2str(k)])
44 end
45 end
```

**Test multiple fields** Set a profile, and evaluate the interpolation. For the case of the highest wavenumber, squash the error when the centre-patch values are all zero.

```

54 for k=1:nPatch/2
55 u0=sin(k*patches.x*2*pi/Len);
56 v0=cos(k*patches.x*2*pi/Len);
57 uvi=patchEdgeInt1([u0(:);v0(:)]);
58 normuError=norm(uvi(:,:,1)-u0)*norm(u0(i0,:));
59 normvError=norm(uvi(:,:,2)-v0)*norm(v0(i0,:));
60 if abs(normuError)+abs(normvError)>2e-13
61     normuError=normuError, normvError=normvError
62     error(['failed double field interpolation k=' num2str(k)])
63 end
64 end

End the for-loop over various geometries.

71 end

```

**Now test spectral interpolation on staggered grid** Must have even number of patches for a staggered grid.

```

79 for nPatch=6:2:20
80 nPatch=nPatch
81 ratio=0.5*rand
82 nSubP=3; % of form 4*N-1
83 Len=10*rand
84 configPatches1(@simpleWavepde,[0,Len],nan,nPatch,-1,ratio,nSubP);
85 kMax=floor((nPatch/2-1)/2)

```

Identify which microscale grid points are  $h$  or  $u$  values.

```

91 uPts=mod( bsxfun(@plus,(1:nSubP)',(1:nPatch)) ,2);
92 hPts=find(1-uPts);
93 uPts=find(uPts);

```

Set a profile for various wavenumbers. The capital letter **U** denotes an array of values merged from both  $u$  and  $h$  fields on the staggered grids.

```

100 fprintf('Single field-pair test.\n')
101 for k=-kMax:kMax

```

```

102 U0=nan(nSubP,nPatch);
103 U0(hPts)=rand*exp(+1i*k*patches.x(hPts)*2*pi/Len);
104 U0(uPts)=rand*exp(-1i*k*patches.x(uPts)*2*pi/Len);
105 Ui=patchEdgeInt1(U0(:));
106 normError=norm(Ui-U0);
107 if abs(normError)>5e-14
108     normError=normError
109     error(['failed single sys interpolation k=' num2str(k)])
110 end
111 end

```

**Test multiple fields** Set a profile, and evaluate the interpolation. For the case of the highest wavenumber zig-zag, squash the error when the alternate centre-patch values are all zero. First shift the  $x$ -coordinates so that the zig-zag mode is centred on a patch.

```

121 fprintf('Two field-pairs test.\n')
122 x0=patches.x((nSubP+1)/2,1);
123 patches.x=patches.x-x0;
124 for k=1:nPatch/4
125     U0=nan(nSubP,nPatch); V0=U0;
126     U0(hPts)=rand*sin(k*patches.x(hPts)*2*pi/Len);
127     U0(uPts)=rand*sin(k*patches.x(uPts)*2*pi/Len);
128     V0(hPts)=rand*cos(k*patches.x(hPts)*2*pi/Len);
129     V0(uPts)=rand*cos(k*patches.x(uPts)*2*pi/Len);
130     UVi=patchEdgeInt1([U0(:);V0(:)]);
131     normuError=norm(UVi(:,1:2:nPatch,1)-U0(:,1:2:nPatch))*norm(U0(i0,2
132         +norm(UVi(:,2:2:nPatch,1)-U0(:,2:2:nPatch))*norm(U0(i0,1:2:nPa
133     normuError=norm(UVi(:,1:2:nPatch,2)-V0(:,1:2:nPatch))*norm(V0(i0,2
134         +norm(UVi(:,2:2:nPatch,2)-V0(:,2:2:nPatch))*norm(V0(i0,1:2:nPa
135     if abs(normuError)+abs(normvError)>2e-13
136         normuError=normuError, normvError=normvError
137         error(['failed double field interpolation k=' num2str(k)])
138     end
139 end

```

End for-loop over patches

146 end

**Finish** If no error messages, then all OK.

157 fprintf ('\nIf you read this, then all tests were passed\n')

## 4.13 patchEdgeInt2test: tests 2D spectral interpolation

Try 99 realisations of random tests.

11 clear all, close all  
 12 global patches  
 13 for realisation=1:99

Choose and configure random sized domains, random sub-patch resolution, random size-ratios, random number of periodic-patches.

19 Lx=1+3\*rand, Ly=1+3\*rand  
 20 nSubP=1+2\*randi(3,1,2)  
 21 ratios=rand(1,2)/2  
 22 nPatch=2+randi(4,1,2)  
 23 configPatches2(@sin,[0 Lx 0 Ly],nan,nPatch,0,ratios,nSubP)

Choose a random number of fields, then generate trigonometric shape with random wavenumber and random phase shift.

29 nV=randi(3)  
 30 [nx,Nx]=size(patches.x);  
 31 [ny,Ny]=size(patches.y);  
 32 u0s=nan(nx,ny,Nx,Ny,nV);  
 33 for iV=1:nV  
 34 kx=randi([0 ceil((nPatch(1)-1)/2)])  
 35 ky=randi([0 ceil((nPatch(2)-1)/2)])  
 36 phix=pi\*rand\*(2\*kx~=nPatch(1))  
 37 phiy=pi\*rand\*(2\*ky~=nPatch(2))

```

38 % generate 2D array via auto-replication
39 u0=sin(2*pi*kx*patches.x(:) /Lx+phix) ...
40 .*sin(2*pi*ky*patches.y(:)'/Ly+phiy);
41 % reshape into 4D array
42 u0=reshape(u0,[nx Nx ny Ny]);
43 u0=permute(u0,[1 3 2 4]);
44 % store into 5D array
45 u0s(:,:,:,:,iV)=u0;
46 end

```

Copy and NaN the edges, then interpolate

```

52 u=u0s; u([1 end],:,:,:,:)=nan; u(:,[1 end],:,:,:)=nan;
53 u=patchEdgeInt2(u(:));

```

If there is an error in the interpolation then abort the script for checking:  
record parameter values and inform.

```

59 err=u-u0s;
60 normerr=norm(err(:))
61 if normerr>1e-12, error('2D interpolation failed'), end
62 end

```

## A Create, document and test algorithms

For developers to create and document the various functions, we use an idea due to Neil D. Lawrence of the University of Sheffield:

- Each class of toolbox functions is located in separate directories in the repository, say **Dir**.
- Create a L<sup>A</sup>T<sub>E</sub>X file **Dir/funs.tex**: establish as one L<sup>A</sup>T<sub>E</sub>X section that `\input{Dir/*.m}`s the files of the functions in the class, example scripts of use, and possibly test scripts, [Table 1](#).
- Each such **Dir/funs.tex** file is to be included from the main L<sup>A</sup>T<sub>E</sub>X file **Doc/equationFreeDoc.tex** so that people can most easily work on one section at a time:
  - put `\include{funs}` into **Doc/equationFreeDoc.tex**;
  - to include we have to use a soft link so at the command line in the directory **Doc** execute `ln -s ../Dir/funs.tex`<sup>2</sup>
- Each toolbox function is documented as a separate subsection, with tests and examples as separate subsections.
- Each function-subsection and test-subsection is to be created as a MATLAB/Octave **Dir/\*.m** file, say **Dir/fun1.m**, so that users simply invoke the function in MATLAB/Octave as usual by `fun1(...)`.

Some editors may need to be told that **fun1.m** is a L<sup>A</sup>T<sub>E</sub>X file. For example, TexShop on the Mac requires one to execute in a Terminal

```
defaults write TeXShop OtherTeXExtensions -array-add "m"
```

- [Table 2](#) gives the template for the **Dir/\*.m** function-subsections. The format for a example/test-subsection is similar.

---

<sup>2</sup>Such soft links are necessary for at least my Mac OSX and hopefully will work for other developers. Further, it has the advantage that auxiliary files are also located in the **Doc** directory.

Table 1: example `Dir/*.tex` file to typeset in the master document a function-subsection, say `fun.m`, and maybe the test/example-subsections.

```

1 % input *.m files for ... Author, date
2 %!TEX root = ../Doc/equationFreeDoc.tex
3 \section{...}
4 \label{sec:...}
5 \localtableofcontents
6 introduction...
7 \input{../Dir/fun.m}
8 \input{../Dir/funExample.m}
9 ...
10 \begin{body}
11 \subsection{To do}
12 ...
13 \subsection{Miscellaneous tests}
14 \input{../Dir/funTest.m}
15 ...
16 \end{body}
```

- Any figures from examples should be generated and then saved for later inclusion with the following (which finally works properly for MATLAB 2017+)

```
set(gcf,'PaperPosition',[0 0 14 10])
print('-depsc2',filename)
```

Include with `\includegraphics[scale=0.85]{filename}`

Table 2: template for a function-subsection `Dir/*.m` file.

```

1 % Short explanation for users typing "help fun"
2 % Author, date
3 %!TEX root = ../Doc/equationFreeDoc.tex
4 %{
5 \subsection{\texttt{...}: ...}
6 \label{sec:...}
7 \localtableofcontents
8 Overview LaTeX explanation.
9 \begin{matlab}
10 %}
11 function ...
12 %{
13 \end{matlab}
14 \paragraph{Input} ...
15 \paragraph{Output} ...
16 \begin{body}
17 Repeated as desired:
18 LaTeX between end-matlab and begin-matlab
19 \begin{matlab}
20 %}
21 Matlab code between \%} and \%{
22 %{
23 \end{matlab}
24 Concluding LaTeX before following final lines.
25 \end{body}
26 %}

```

## B Aspects of developing a ‘toolbox’ for patch dynamics

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This appendix documents sketchy further thoughts on aspects of the development.

### B.1 Macroscale grid

The patches are to be distributed on a macroscale grid: the  $j$ th patch ‘centred’ at position  $\vec{X}_j \in \mathbb{X}$ . In principle the patches could move, but let’s keep them fixed in the first version. The simplest macroscale grid will be rectangular (`meshgrid`), but we plan to allow a deformed grid to secondly cater for boundary fitting to quite general domain shapes  $\mathbb{X}$ . And plan to later allow for more general interconnect networks for more topologies in application.

### B.2 Macroscale field variables

The researcher/practitioner has to know an appropriate set of macroscale field variables  $\vec{U}(t) \in \mathbb{R}^{d_{\vec{U}}}$  for each patch. For example, first they might be a simple average over a core of a patch of all of the micro-field variables;

second, they might be a subset of the average micro-field variables; and third in general the macro-variables might be a nonlinear function of the micro-field variables (such as temperature is the average speed squared). The core might be just one point, or a sizeable fraction of the patch.

The mapping from microscale variable to macroscale variables is often termed the restriction.

In practice, users may not choose an appropriate set of macro-variables, so will eventually need to code some diagnostic to indicate a failure of the assumed closure.

### B.3 Boundary and coupling conditions

The physical domain boundary conditions are distinct from the conditions coupling the patches together. Start with physical boundary conditions of periodicity in the macroscale.

Second, assume the physical boundary conditions are that the macro-variables are known at macroscale grid points around the boundary. Then the issue is to adjust the interpolation to cater for the boundary presence and shape. The coupling conditions for the patches should cater for the range of Robin-like boundary conditions, from Dirichlet to Neumann. Two possibilities arise: direct imposition of the coupling action ([Roberts & Kevrekidis 2007](#)), or control by the action.

Third, assume that some of the patches have some edges coincident with the boundary of the macroscale domain  $\mathbb{X}$ , and it is on these edges that macroscale physical boundary conditions are applied. Then the interpolation from the core of these edge patches is the same as the second case of prescribed boundary macro-variables. An issue is that each boundary patch should be big enough to cater for any spatial boundary layers transitioning from the applied boundary condition to the interior slow evolution.

Alternatively, we might have the physical boundary condition constrain the interpolation between patches.

Often microscale simulations are easiest to write when ‘periodic’ in microscale space. To cater for this we should also allow a control at perhaps the quartiles of a micro-periodic simulator.

## B.4 Mesotime communication

Since communication limits large scale parallelism, a first step in reducing communication will be to implement only updating the coupling conditions when necessary. Error analysis indicates that updating on times longer the microscale times and shorter than the macroscale times can be effective ([Bunder et al. 2016](#)). Implementations can communicate one or more derivatives in time, as well as macroscale variables.

At this stage we can effectively parallelise over patches: first by simply using Matlab’s `parfor`. Probably not using a GPU as we probably want to leave GPUs for the black box to utilise within each patch.

## B.5 Projective integration

To take macroscale time steps, invoke several possible projective integration schemes: simple Euler projection, Heun-like method, etc ([Samaey et al. 2010](#)). Need to decide how long a microscale burst needs to be.

Should not need an implicit scheme as the fast dynamics are meant to be only in the micro variables, and the slow dynamics only in the macroscale variables. However, it could be that the macroscale variables have fast oscillations and it is only the amplitude of the oscillations that are slow. Perhaps need to detect and then fix or advise.

A further stage is to implement a projective integration scheme for stochastic macroscale variables: this is important because the averaging over a core of microscale roughness will almost invariably have at least some stochastic legacy effect. [Calderon \(2007\)](#) did some useful research on stochastic projective intergration.

## B.6 Lift to many internal modes

In most problems the number of macroscale variables at any given position in space,  $d_{\vec{U}}$ , is less than the number of microscale variables at a position,  $d_{\vec{u}}$ ; often much less ([Kevrekidis & Samaey 2009](#), e.g.). In this case, every time we start a patch simulation we need to provide  $d_{\vec{u}} - d_{\vec{U}}$  data at each position in the patch: this is lifting. The first methodology is to first guess, then run repeated short bursts with reinitialisation, until the simulation reaches a slow manifold. Then run the real simulation.

If the time taken to reach a local quasi-equilibrium is too long, then it is likely that the macroscale closure is bad and the macroscale variables need to be extended.

A second step is to cater for cases where the slow manifold is stochastic or is surrounded by fast waves: when it is hard to detect the slow manifold, or the slow manifold is not attractive.

## B.7 Macroscale closure

In some circumstances a researcher/practitioner will not code the appropriately set of macroscale variables for a complete closure of the macroscale. For example, in thin film fluid dynamics at low Reynolds number the only macroscale variable is the fluid depth; however, at higher Reynolds number, circa ten, the inertia of the fluid becomes important and the macroscale variables must additionally include a measure of the mean lateral velocity/momenta ([Roberts & Li 2006](#), e.g.).

At some stage we need to detect any flaw in the closure, and perhaps suggest additional appropriate macroscale variables, or at least their characteristics. Indeed, a poor closure and a stochastic slow manifold are really two faces of the same problem: the problem is that the chosen macroscale variables do not have a unique evolution in terms of themselves. A good resolution of the issue will account for both faces.

## B.8 Exascale fault tolerance

Matlab is probably not an appropriate vehicle to deal with real exascale faults. However, we should cater by coding procedures for fault tolerance and testing them at least synthetically. Eventually provide hooks to a user routine to be invoked under various potential scenarios. The nature of fault tolerant algorithms will vary depending upon the scenario, even assuming that each patch burst is executed on one CPU (or closely coupled CPUS): if there are much more CPUs than patches, then maybe simply duplicate all patch simulations; if much less CPUs than patches, then an asynchronous scheduling of patch bursts should effectively cater for recomputation of failed bursts; if comparable CPUS to patches, then more subtle action is needed.

Once mesotime communication and projective integration is provided, a recomputation approach to intermittent hardware faults should be effective because we then have the tools to restart a burst from available macroscale data. Should also explore proceeding with a lower order interpolation that misses the faulty burst—because an isolated lower order interpolation probably will not affect the global order of error (it does not in approximating some boundary conditions ([Gustafsson 1975](#), [Svard & Nordstrom 2006](#))

## B.9 Link to established packages

Several molecular/particle/agent based codes are well developed and used by a wide community of researchers. Plan to develop hooks to use some such codes as the microscale simulators on patches. First, plan to connect to LAMMPS ([Plimpton et al. 2016](#)). Second, will evaluate performance, issues, and then consider what other established packages are most promising.

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