Equation-Free function toolbox for Matlab/Octave: Summary User Manual

A. J. Roberts[*] John Maclean[†] J. E. Bunder[‡] et al.[§]

February 26, 2019

Abstract

This 'equation-free toolbox' empowers the computer-assisted analysis of complex, multiscale systems. Its aim is to enable you to use microscopic simulators to perform system level tasks and analysis. 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.

Contents

[*]School of Mathematical Sciences, University of Adelaide, South Australia. http://www.maths.adelaide.edu.au/anthony.roberts, http://orcid.org/0000-0001-8930-1552

[†]School of Mathematical Sciences, University of Adelaide, South Australia. http://www.adelaide.edu.au/directory/john.maclean

[‡]School of Mathematical Sciences, University of Adelaide, South Australia. mailto:judith.bunder@adelaide.edu.au, http://orcid.org/0000-0001-5355-2288

[§]Appear here for your contribution.

1 Introduction

Subsubsection contents

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 micro-field variables could be in $\mathbb{R}^p$ for any $p = 1, 2, \ldots, \infty$.

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. **??** outlines some details for contributors.

2 Quick start

Section contents

This section may be used in conjunction with the many examples in later sections to help apply the toolbox functions to a particular problem, or to assist in distinguishing between the various functions.

2.1 Cheat sheet: Projective Integration

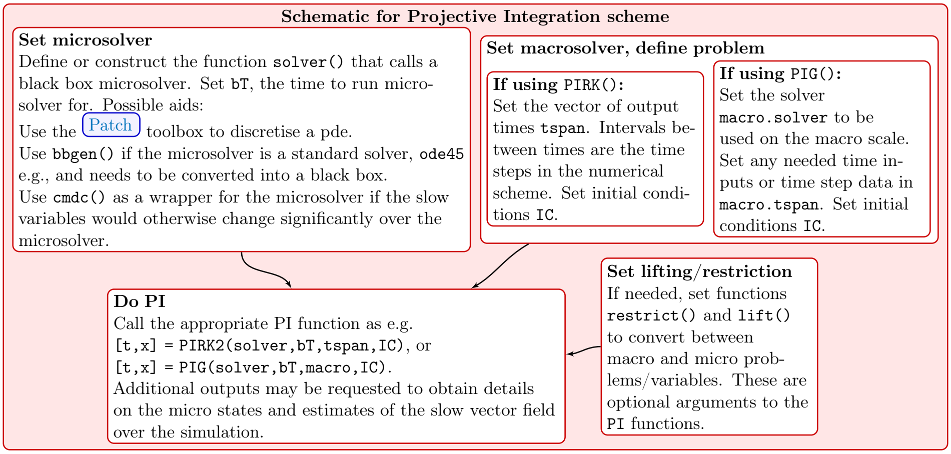
This section pertains to the Projective Integration (PI) methods of Section 3. The PI approach is to greatly accelerate computations of a system exhibiting multiple time scales.

The PI toolbox presents several 'main' functions that could separately be called to perform PI, as well as several optional wrapper functions that may be called. This section helps to distinguish between the top-level PI functions, and helps to tell which of the optional functions may be needed at a glance. For full details on each function refer to Section 3.

The cheat sheet consists of two flow charts. For an overview of constructing a PI simulation, see Figure 1. For a rough guide as to which of the top-level PI functions should be used, refer to Figure 2.

2.2 Cheat sheet: constructing patches

This section pertains to the Patch approach to discretising PDEs of Section 3.



Schematic for Projective Integration scheme

Set microsolver
Define or construct the function `solver()` that calls a black box microsolver. Set `bT`, the time to run microsolver for. Possible aids:
Use the Patch toolbox to discretise a pde.
Use `bbgen()` if the microsolver is a standard solver, `ode45` e.g., and needs to be converted into a black box.
Use `cmdc()` as a wrapper for the microsolver if the slow variables would otherwise change significantly over the microsolver.

Set macrosolver, define problem

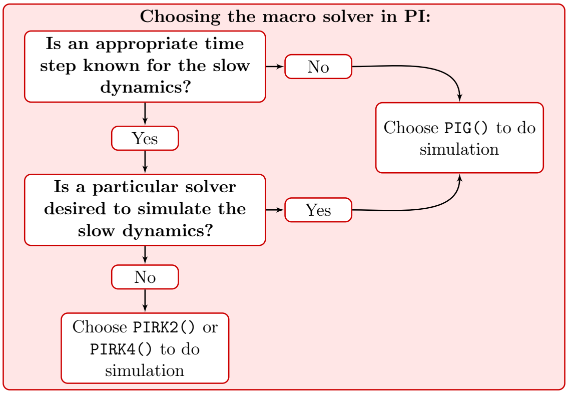
If using `PIRK()`:
Set the vector of output times `tspan`. Intervals between times are the time steps in the numerical scheme. Set initial conditions `IC`.

If using `PIG()`:
Set the solver `macro.solver` to be used on the macro scale. Set any needed time inputs or time step data in `macro.tspan`. Set initial conditions `IC`.

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

Do PI
Call the appropriate PI function as e.g.
`[t,x] = PIRK2(solver,bT,tspan,IC)`, or
`[t,x] = PIG(solver,bT,macro,IC)`.
Additional outputs may be requested to obtain details on the micro states and estimates of the slow vector field over the simulation.

Figure 1



Choosing the macro solver in PI:

Is an appropriate time step known for the slow dynamics?

Choose `PIG()` to do simulation

Is a particular solver desired to simulate the slow dynamics?

Choose `PIRK2()` or `PIRK4()` to do simulation

Figure 2

The Patch toolbox requires that one configure patches, couple the patches and interface the coupled patches with a time integrator. For an overview of the chief functions involved and their interactions, see Figure 3.

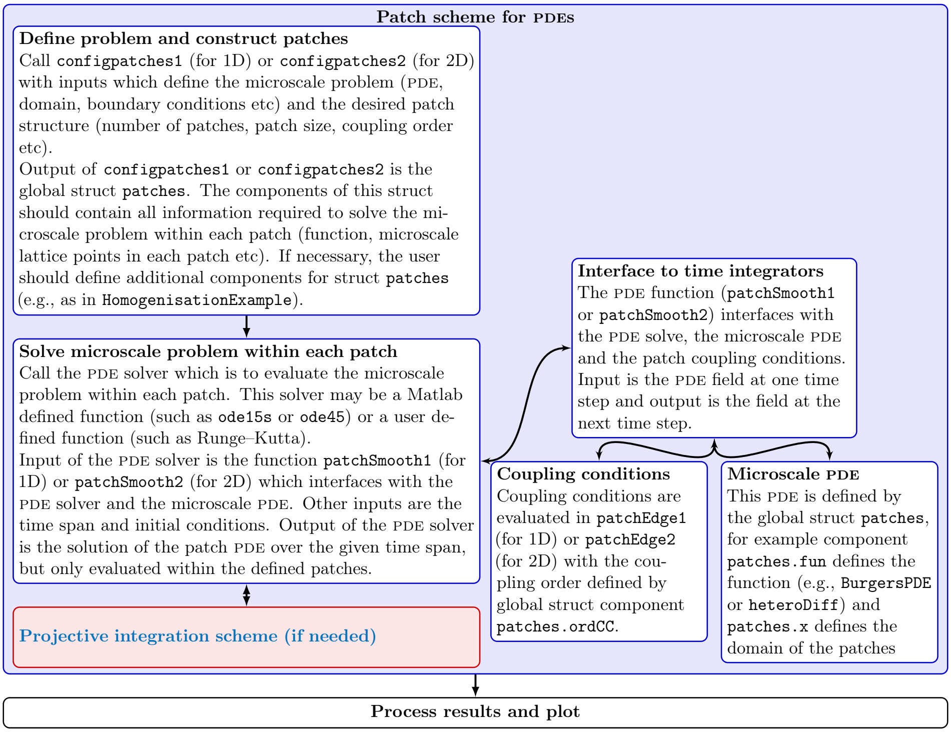

Patch scheme for PDEs
Define problem and construct patches
Call `configpatches1` (for 1D) or `configpatches2` (for 2D) with inputs which define the microscale problem (PDE, domain, boundary conditions etc) and the desired patch structure (number of patches, patch size, coupling order etc).
Output of `configpatches1` or `configpatches2` is the global struct `patches`. The components of this struct should contain all information required to solve the microscale problem within each patch (function, microscale lattice points in each patch etc). If necessary, the user should define additional components for struct `patches` (e.g., as in `HomogenisationExample`).
Solve microscale problem within each patch
Call the PDE solver which is to evaluate the microscale problem within each patch. This solver may be a Matlab defined function (such as `ode15s` or `ode45`) or a user defined function (such as Runge–Kutta).
Input of the PDE solver is the function `patchSmooth1` (for 1D) or `patchSmooth2` (for 2D) which interfaces with the PDE solver and the microscale PDE. Other inputs are the time span and initial conditions. Output of the PDE solver is the solution of the patch PDE over the given time span, but only evaluated within the defined patches.
Interface to time integrators
The PDE function (`patchSmooth1` or `patchSmooth2`) interfaces with the PDE solve, the microscale PDE and the patch coupling conditions. Input is the PDE field at one time step and output is the field at the next time step.
Coupling conditions
Coupling conditions are evaluated in `patchEdge1` (for 1D) or `patchEdge2` (for 2D) with the coupling order defined by global struct component `patches.ordCC`.
Microscale PDE
This PDE is defined by the global struct `patches`, for example component `patches.fun` defines the function (e.g., `BurgersPDE` or `heteroDiff`) and `patches.x` defines the domain of the patches
Projective integration scheme (if needed)
Process results and plot

Figure 3

3 Projective integration of deterministic ODEs

Subsubsection contents

This section provides some good projective integration functions (Gear & Kevrekidis 2003*a*,*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 3.2 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.
- '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.

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

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

3.1 `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.

```
function [x, tms, xms, rm, svf] = PIRK2(microBurst, 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 3.1.1 as a basic template of how to use.

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

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

  - Inputs: `tStart`, the start time of a burst of simulation; `xStart`, the row n-vector of the starting state; `bT`, 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 microBurst to relax the fast variables to the slow manifold.

- `tSpan` is an ℓ-vector of times at which the user requests output, of which the first element is always the initial time. `PIRK2()` does not use adaptive time stepping; the macroscale time steps are (nearly) the steps between elements of `tSpan`.

- `x0` is an n-vector of initial values at the initial time `tSpan(1)`. Elements of `x0` may be `NaN`: they are included in the simulation and output, and often represent boundaries in space fields.

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

1. a macroscale time step, $\Delta =$ `diff(tSpan)`, such that $\alpha\Delta \approx \sqrt{6\varepsilon}$, and
2. a microscale burst length, $\delta =$ `bT` $\gtrsim \frac{1}{\beta}\log(\beta\Delta)$ (see Figure 4).

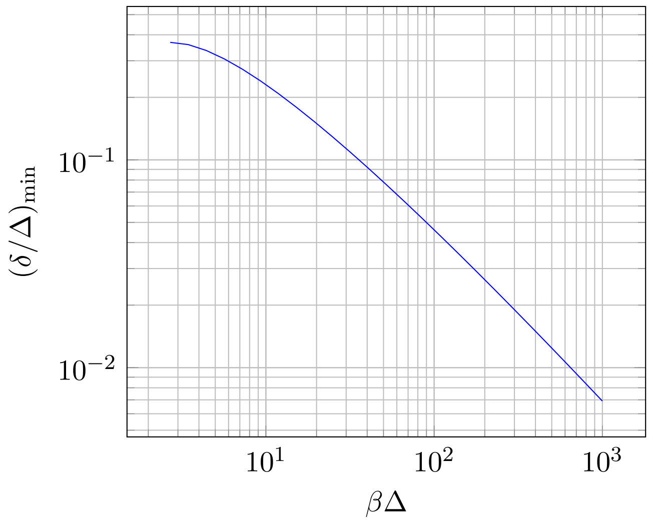
Output If there are no output arguments specified, then a plot is drawn of the computed solution `x` versus `tSpan`.

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

Figure 4: Need macroscale step Δ such that $|\alpha\Delta| \lesssim \sqrt{6\varepsilon}$ for given relative error ε and slow rate α, and then $\delta/\Delta \gtrsim \frac{1}{\beta\Delta}\log\beta\Delta$ determines the minimum required burst length δ for given fast rate β.



- `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 microBurst required by the Projective Integration method during the calculation of the macrostep:
  - `rm.t` is a column vector of microscale times; and
  - `rm.x` is the array of corresponding burst states.

  The states `rm.x` do not have the same physical interpretation as those in `xms`; the `rm.x` are required in order to estimate the slow vector field during the calculation of the Runge–Kutta increments, and do not in general resemble the true dynamics.
- `svf`, optional, a struct containing the Projective Integration estimates

of the slow vector field.

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

3.1.1 If no arguments, then execute an example

```
if nargin==0
```

Example code for Michaelis–Menton dynamics The Michaelis–Menten enzyme kinetics is expressed as a singularly perturbed system of differential equations for $x(t)$ and $y(t)$ (encoded in function `MMburst` in the next paragraph):

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

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

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

Upon finishing execution of the example, exit this function.

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

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

```
function [ts, xs] = MMburst(ti, xi, bT)
    dMMdt = @(t,x) [ -x(1)+(x(1)+0.5)*x(2)
          1/epsilon*( x(1)-(x(1)+1)*x(2) ) ];
    [ts, xs] = ode23(dMMdt, [ti ti+bT], xi);
end
```

3.2 egPIMM: Example projective integration of Michaelis–Menton kinetics

Subsection contents

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

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

As illustrated in Figure 6, the slow variable $x(t)$ evolves on a time scale of one, whereas the fast variable $y(t)$ evolves on a time scale of the small parameter ϵ.

3.2.1 Invoke projective integration

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

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

First, Section 3.2.2 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 2ϵ, and starting from the initial condition for the Michaelis–Menten system of $(x(0), y(0)) = (1, 0)$ (off the slow manifold).

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

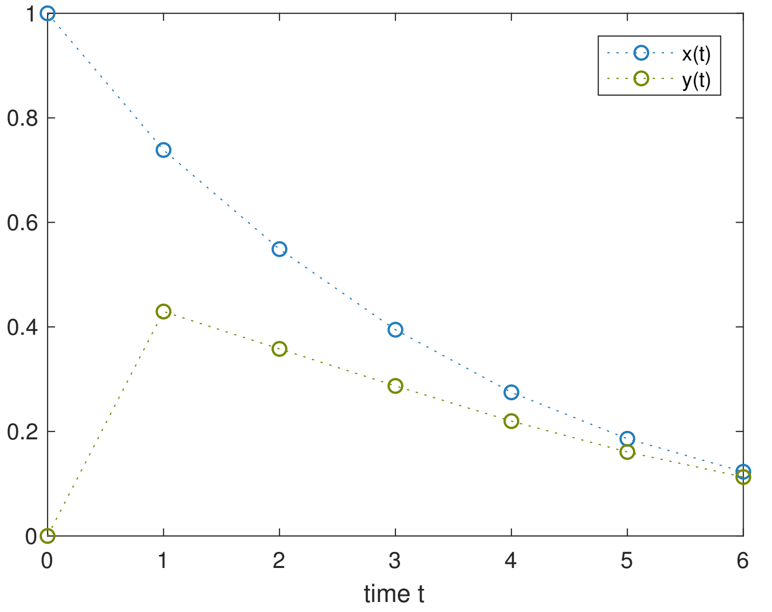
Figure 5 plots the macroscale results showing the long time decay of the Michaelis–Menten system on the slow manifold. **?** [§4] used this system as an example of their analysis of the convergence of Projective Integration.

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 5). To see the initial transient attraction to the slow manifold we plot some microscale data in Figure 6. Two further output variables provide this microscale burst information.

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

Figure 6 plots the macroscale and microscale results—also showing that the initial burst is by default twice as long. Observe the slow variable $x(t)$ is also affected by the initial transient which indicates that other schemes which 'freeze' slow variables are less accurate.

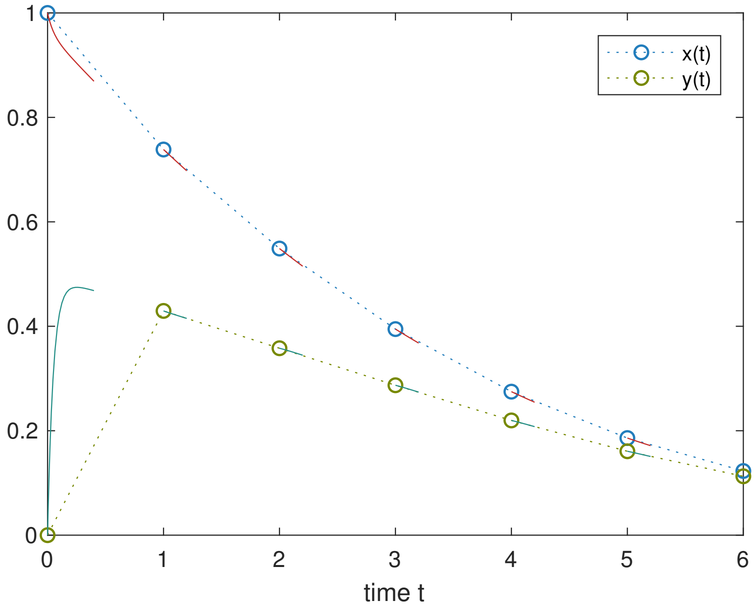
Figure 5: Michaelis–Menten enzyme kinetics simulated with the projective integration of `PIRK2()`: macroscale samples.



Optional: simulate backwards in time Figure 7 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 3ϵ.

```
ts = 0:-1:-5
[xs,tMicro,xMicro] = PIRK2(@MMburst, 3*epsilon, ts, 0.2*[1;1]);
figure, plot(ts,xs,'o:',tMicro,xMicro)
xlabel('time t'), legend('x(t)','y(t)')
```

Figure 6: 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.

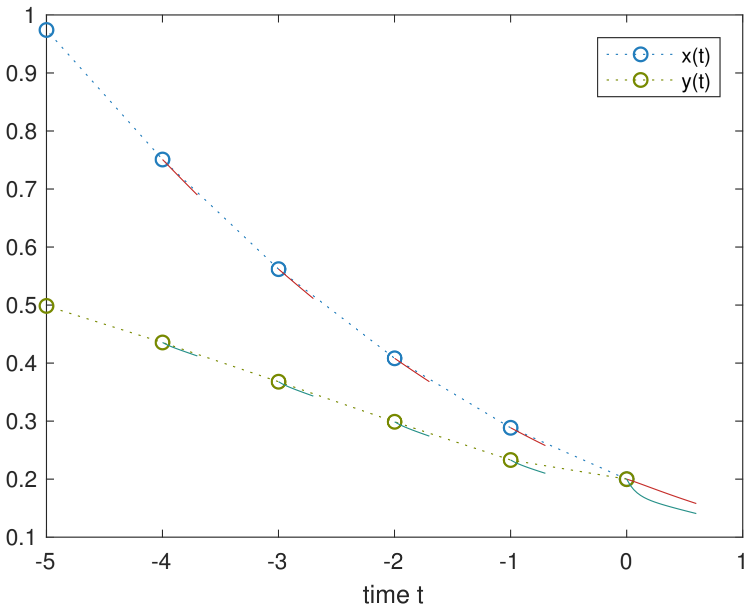


3.2.2 Code a burst of Michaelis–Menten enzyme kinetics

Say use `ode23()` to integrate a burst of the differential equations for the Michaelis–Menten enzyme kinetics. Code differential equations in function `dMMdt` with variables x = `x(1)` and y = `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.

```
function [ts, xs] = MMburst(ti, xi, bT)
    global epsilon
    dMMdt = @(t,x) [ -x(1)+(x(1)+0.5)*x(2)
          1/epsilon*( x(1)-(x(1)+1)*x(2) ) ];
    [ts, xs] = ode23(dMMdt, [ti ti+bT], xi);
end
```

Figure 7: Michaelis–Menten 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 $\epsilon = 0.1$.



3.3 `PIG()`: Projective Integration via a General macroscale integrator

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

By default, `PIG()` uses 'constraint-defined manifold computing' for the microscale simulations. This algorithm, developed in Gear et al. (2005), Zagaris et al. (2012), Unlike the `PIRKn` functions, `PIG()` does not 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 micro-burst simulator. 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

- either very stiff problems, in which the burst length of the micro-burst can be short,
- or the 'constraint defined manifold' based micro-burst provided by `cdmc()`, that attempts to project the variables onto the slow manifold without affecting the time.

```
% function [t,x,tms,xms,svf] = PIG(macroInt,microBurst,tSpan,x0,restr
function varargout = PIG(macroInt,microBurst,tSpan,x0,varargin)
```

Inputs:

- `microBurst()` is a function that produces output from the user-specified code for a burst of micro-scale simulation. The function must know how long a burst it is to use. Usage

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

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

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

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

  `[ts,xs] = macroInt(f,tSpan,x0)`

  where function `f(t,x)` notionally evaluates the time derivatives $d\vec x/dt$ at 'any' time; `tSpan` is either the macro-time interval, or the vector of times at which a macroscale value is to be returned; and `x0` are the initial values of $\vec x$ at time `tSpan(1)`. Then the ith *row* of `xs`, `xs(i,:)`, is to be the vector $\vec{x}(t)$ at time $t =$ `ts(i)`. Remember that in `PIG()` the function `f(t,x)` is to be estimated by Projective Integration burst.

- `tSpan`, a vector of times at which the user requests output, of which the first element is always the initial time. If `macroInt` can adaptively select time steps (e.g., `ode45`), then `tSpan` can consist of an initial and final time only.
- `x0`, the N-vector of initial values at the initial time `tSpan(1)`.

Optional Inputs: If the microscale state and macroscale state are of different dimensions, then functions must be provided to convert between them.

- `restrict()`, a function that takes an n-dimensional microscale state and returns an N-dimensional macroscale state.
- `lift()`, a function that converts an input N-dimensional macroscale state to an n-dimensional microscale state.
- `nocdmcflag`. Any variable supplied as a seventh input to `PIG()` will turn off the default constraint-defined manifold computing behaviour. For clarity, it is suggested to use a string, e.g. `nocdmcflag = 'flag cdmc off'`. If this flag is needed but the lifting /restriction functions are not, the

Output If there are no output arguments specified, then a plot is drawn of the computed solution `x` versus `t`. Most often you would only store the first two output results of `PIG()`, via say `[t,x] = PIG(...)`.

- `t`, an ℓ-vector of times at which `macroInt` produced results.
- `x`, an $\ell \times n$ array of the computed solution: the ith *row* of `x`, `x(i,:)`, is to be the vector $\vec{x}(t)$ at time $t =$ `t(i)`.

  However, microscale details of the underlying Projective Integration computations may be helpful, and so `PIG()` some 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.
- `svf`, optional, a struct containing the Projective Integration estimates of the slow vector field.
  - `svf.t` is a 2ℓ dimensional column vector containing all times at which the Projective Integration scheme is extrapolated along microsolver data to form a macrostep.
  - `svf.dx` is a $2\ell\times n$ array containing the estimated slow vector field.

3.3.1 If no arguments, then execute an example

```
if nargin==0
```

As a basic example, consider a singularly perturbed system of differential equations for $\vec x(t)=(x_1(t),x_2(t))$:

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

With initial conditions $\vec x(0)=(1,0)$, the following code computes and plots a solution of the system over time $0\le t\le 6$ for parameter $\epsilon=10^{-3}$.

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

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

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

```
bT = 2*epsilon*log(1/epsilon)
microBurst = @(tb0,xb0) ode23(dxdt,[tb0 tb0+bT],xb0);
```

Third, suppose that the macroscale simulation is to be of `x_1` only, and code a function to `restrict` the variables to only the macroscale, and a function (called `lift`) to return the macroscale variables to a compatible microscale state.

```
lif = @(x) [x; 0.5];
res = @(x) x(1);
```

Fourth, invoke `PIG` to use `ode23()`, say, on the macroscale slow evolution. Integrate the micro-bursts over $0 \leq t \leq 6$ from initial condition $\vec{x} = (1, 0)$. (You could set `tSpan=[0 -6]` to integrate backwards in time with forward bursts.)

```
tSpan = [0 6];
[ts,xs,tms,xms] = PIG('ode23',microBurst,tSpan,1, res, lif);
```

Plot output of this projective integration.

```
figure, plot(ts,xs,'o:',tms,xms,'.')
title('Projective integration of singularly perturbed ODE')
xlabel('time t'), legend('x_1(t)','micro bursts of x_1(t)', 'micro bu
```

Upon finishing execution of the example, exit this function.

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

3.4 PIRK4(): projective integration of fourth order accuracy

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

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

See Section 3.1 as the inputs and outputs are the same as `PIRK2()`.

If no arguments, then execute an example

```
if nargin==0
```

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

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

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

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

Upon finishing execution of the example, exit this function.

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

Example function code for a burst of ODEs Integrate a burst of length bT of the ODEs for the Michaelis–Menten enzyme kinetics at parameter ϵ inherited from above. Code ODEs in function dMMdt with variables $x =$ x(1) and $y =$ x(2). Starting at time ti, and state xi (row), we here simply use ode23 to integrate in time.

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

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

3.4.1 `cdmc()`

`cdmc()` iteratively applies the micro-burst 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.

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

Input

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

Output

- `ts`, a vector of times. `tout(end)` will equal `t`.
- `xs`, an array of state estimates produced by `microBurst()`.

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

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

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

3.5 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.

```
clear
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,

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

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

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

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

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

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

```
dt = 0.001;
bT = 0.05;
```

As a rule of thumb, the time steps `dt` should satisfy $\texttt{dt} \leq 1/|\texttt{fastband}(1)|$ and the time to simulate with each application of the microsolver, `micro.bT`, should be larger than or equal to $1/|$`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

```
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.

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

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

```
tSpan=0: 1 : 30;
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.

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

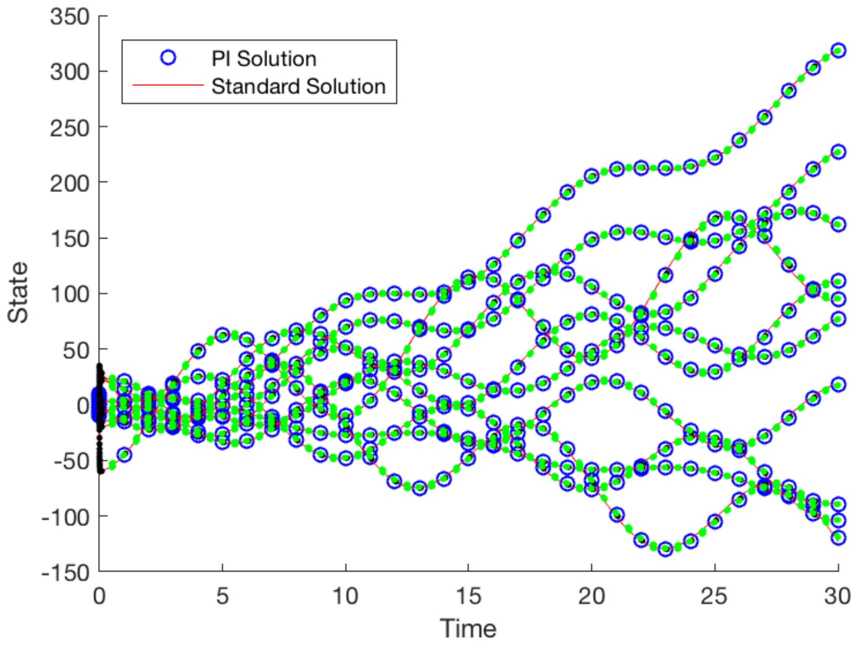
For verification, we also compute the trajectories using a standard solver.

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

Figure 8 plots the output.

```
tmsr = rm.t; xmsr = rm.x;
clf()
hold on
PI_sol=plot(tSpan,x,'bo');
```

Figure 8: Demonstration of PIRK4(). From initial conditions, the system rapidly trannsitions 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.



```
std_sol=plot(tt,ode45x,'r');
plot(tms,xms,'k.');
plot(tmsr,xmsr,'g.');
legend([PI_sol(1),std_sol(1)],'PI Solution',...
    'Standard Solution','Location','NorthWest')
xlabel('Time');
ylabel('State');
```

Save plot to a file.

```
set(gcf,'PaperPosition',[0 0 14 10])
```

```
print('-depsc2','PIRK')
```

3.6 Example: Projective Integration using General macrosolvers

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

```
clear all, close all
```

Set time scale separation and model.

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

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

```
bT = epsilon*log(1/epsilon);
microBurst = @(tb0, xb0) ode45(dxdt,[tb0 tb0+bT],xb0);
```

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

```
x0 = [1 1.4];
tSpan=[0 15];
```

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.

```
tic
[ts,xs,tms,xms] = PIG('ode45',microBurst,tSpan,x0);
tPIGusingODE45asMacro = toc
tic
```

```
[t45,x45] = ode45(dxdt,tSpan,x0);
tODE45alone = toc
```

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

```
figure
h = plot(ts,xs,'o', t45,x45,'-', tms,xms,'.');
legend(h(1:2:5),'PI Solution','ode45 Solution','PI microsolver')
xlabel('Time'), ylabel('State')

figure
h = plot(ts,xs,'o', t45,x45,'-');
legend(h([1 3]),'PI Solution','ode45 Solution')
xlabel('Time'), ylabel('State')
set(gcf,'PaperPosition',[0 0 14 10]), print('-depsc2','PIGExample')
```

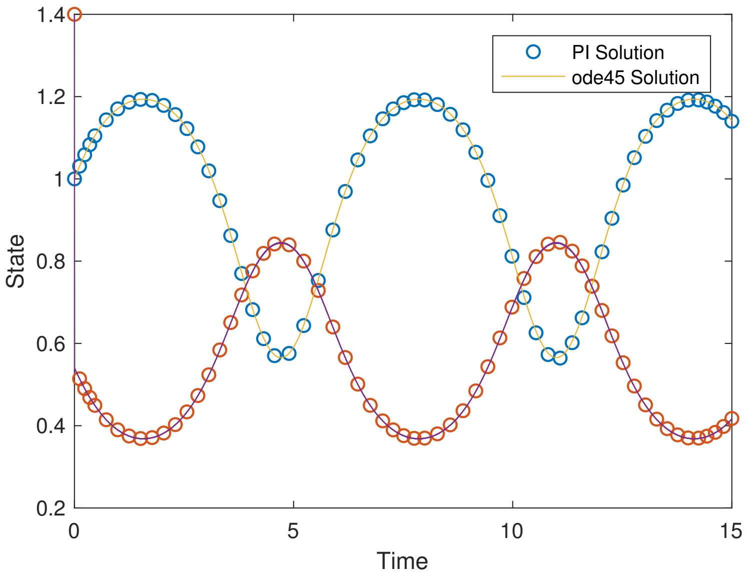
Figure 9 plots the output.

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

  But if the problem is insufficiently stiff (larger ϵ), then `PIG()` produces nonsense. This nonsense is overcome by `cdmc()` (Section 3.7).

- The mildly stiff problem in Section 3.5 may be efficiently solved by a standard solver (e.g., `ode45()`). The stiff but low dimensional problem in this example can be solved efficiently by a standard stiff solver (e.g., `ode15s()`). The real advantage of the Projective Integration schemes is in high dimensional stiff problems, that cannot be efficiently solved by most standard methods.

Figure 9: Accurate simulation of a stiff nonautonomous system by PIG(). The microsolver is called on-the-fly by the macrosolver `ode45`.



3.7 Explore: Projective Integration using constraint-defined manifold computing

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

```
clear all, close all
```

Set a weak time scale separation, and model.

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

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

```
bT = epsilon*log(1/epsilon);
microBurst = @(tb0,xb0) ode45(dxdt,[tb0 tb0+bT],xb0);
```

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

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

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

```
[nt,nx] = PIG('ode45',microBurst,tSpan,x0,[],[],'no cdmc');
[ct,cx] = PIG('ode45',microBurst,tSpan,x0);
[t45,x45] = ode45(dxdt,tSpan([1 end]),x0);
```

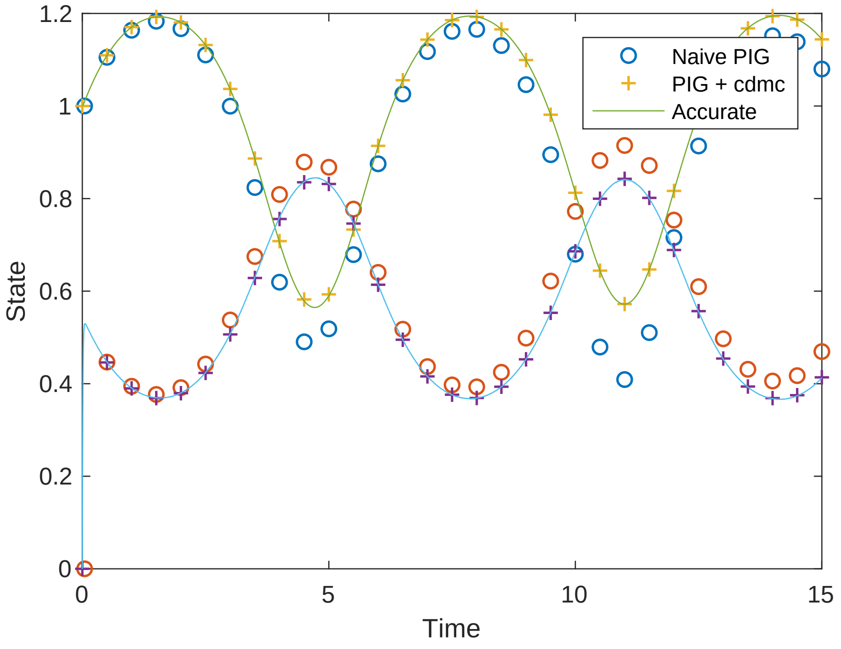
Figure 10 plots the output.

```
figure
h = plot(nt,nx,'rx', ct,cx,'bo', t45,x45,'-');
legend(h(1:2:5),'Naive PIG','default: PIG + cdmc','Accurate')
xlabel('Time'), ylabel('State')
set(gcf,'PaperPosition',[0 0 14 10]), print('-depsc2','PIGExplore')
```

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[1] to worsen the error in both schemes. This example reflects a general principle, that most Projective Integration 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.

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

Figure 10: Accurate simulation of a weakly stiff non-autonomous system by `PIG()` using cdmc(), and an inaccurate solution using a naive application of `PIG()`.



3.8 To do/discuss

- 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 with a little fiddling. Then output at each user-requested coarse time is the end point of an application of the microsolver - better predictions for fast variables.
- Can maybe implement microsolvers that terminate a burst when the fast dynamics have settled using, for example, the 'Events' function

handle in ode23.

4 Patch scheme for given microscale discrete space system

Subsubsection contents

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 structure 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 **????** 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

Subsubsection contents

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

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

Input If invoked with no input arguments, then executes an example of simulating Burgers' PDE—see ?? 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 $geq - 1$.
- `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` $\times$ `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.

4.2 `patchSmooth1()`: interface to time integrators

Subsubsection contents

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 using the previously established global struct `patches`.

```
function dudt=patchSmooth1(t,u)
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.

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

Subsubsection contents

Couples 1D patches across 1D space by computing their edge values from macroscale interpolation patch core averging. This function is primarily used by `patchSmooth1` but is also useful for user graphics. Consequently a spatially discrete system could be integrated in time via the patch or gap-tooth scheme (Roberts & Kevrekidis 2007). Assumes that the core averaged structure is *smooth* so that these averages are sensible macroscale variables, and patch edge values are determined by macroscale interpolation of the core averaged values (**?**). Communicate patch-design variables via the global struct `patches`.

```
function u=patchEdgeInt1(u)
global patches
```

Input

- `u` is a vector of length `nSubP` $\cdot$ `nPatch` $\cdot$ `nVars` where there are `nVars` field values at each of the points in the `nSubP` $\times$ `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 integer ≥ -1.
  - `.alt` in $\{0, 1\}$ is one for staggered grid (alternating) interpolation.
  - `.Cwtsr` and `.Cwtsl` define the coupling.

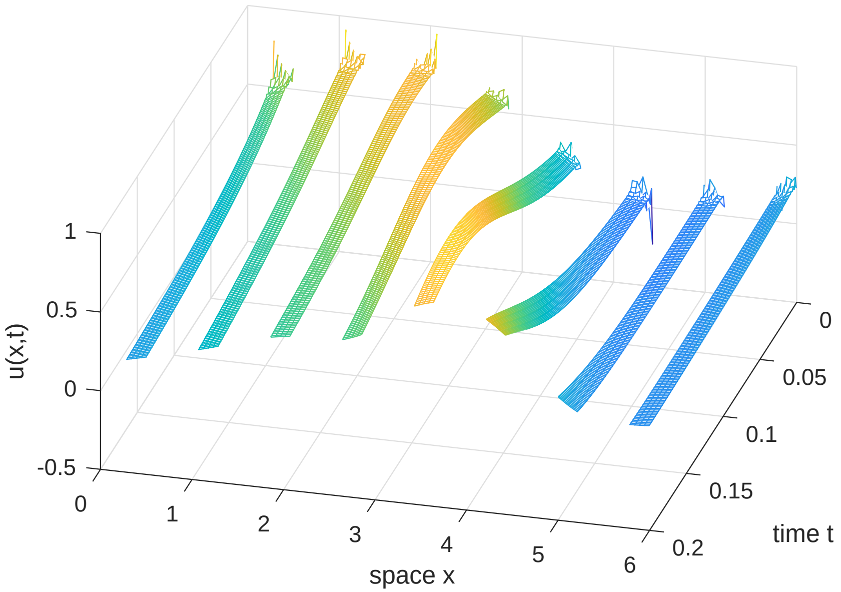
Output

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

4.4 `BurgersExample`: simulate Burgers' PDE on patches

Subsection contents

Figure 11: 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.



?? 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 11), 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

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 2π-periodic domain, with eight patches, each patch of half-size ratio 0.2, with seven points within each patch, and say fourth order interpolation provides edge-values that couple the patches.

```
clear all
global patches
nPatch = 8
ratio = 0.2
nSubP = 7
interpOrd = 4
Len = 2*pi
configPatches1(@burgersMap,[0 Len],nan,nPatch,interpOrd,ratio,nSubP);
```

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

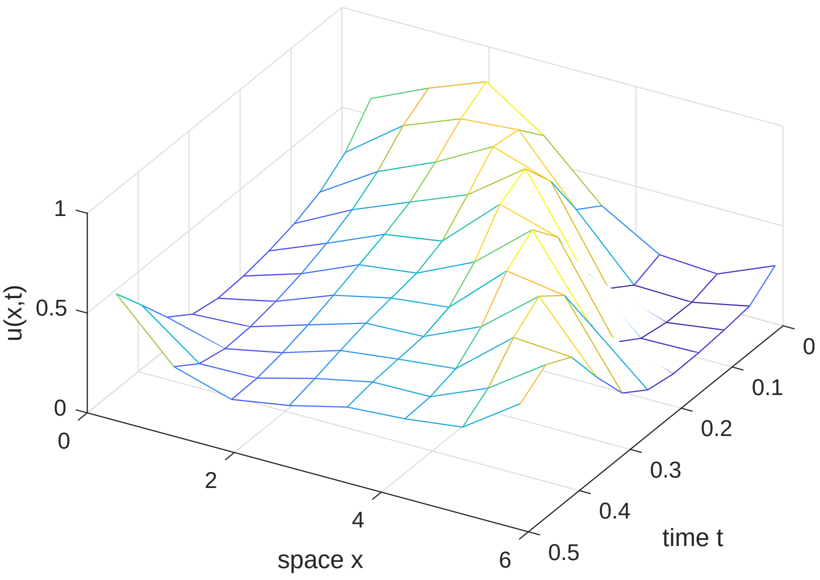
```
u0 = 0.4*(1+sin(patches.x))+0.1*randn(size(patches.x));
[ts,us] = burgerBurst(0,u0,0.2);
```

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

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

Use projective integration Around the micro-scale burst `burgerBurst()`, wrap the projective integration function `PIRK2()` of Section 3.1. Figure 12 shows the macroscale prediction of the patch centre values on macro-scale time-steps.

Figure 12: macro-scale space-time field $u(x,t)$ in a basic projective integration of the patch scheme applied to the micro-scale Burgers' map.



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

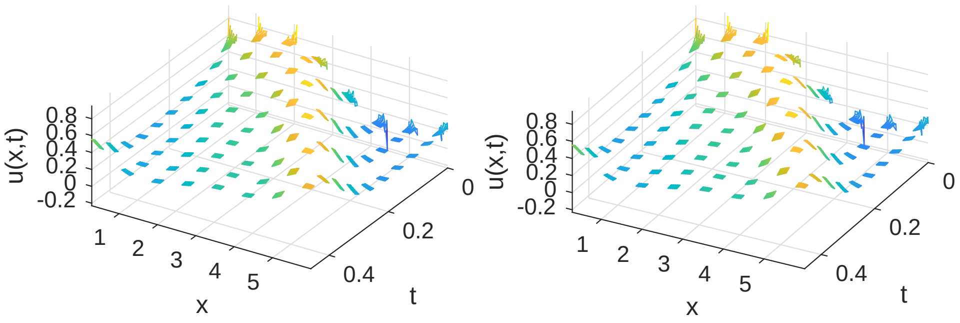
Mark that edge of patches are not to be used in the projective extrapolation by setting initial values to NaN.

```
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.

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

Figure 13: the field $u(x, t)$ during each of the microscale bursts used in the projective integration. View this stereo pair cross-eyed.



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

Plot the macroscale predictions of the mid-patch values to give the macroscale mesh of Figure 12.

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

Then plot the microscale mesh of the microscale bursts shown in Figure 13 (a stereo pair). The details of the fine microscale mesh are almost invisible.

```
figure(3),clf
for k = 1:2, subplot(2,2,k)
  mesh(tss,xs(:),uss')
  ylabel('x'),xlabel('t'),zlabel('u(x,t)')
  axis tight, view(126-4*k,50)
end
set(gcf,'paperposition',[0 0 17 12])
```

```
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).

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

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

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

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

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

```
  us = nan(ndt+1,numel(ui));
  us(1,:) = reshape(ui,1,[]);
  for j = 1:ndt
    ui = patchSmooth1(ts(j),ui);
    us(j+1,:) = reshape(ui,1,[]);
  end
```

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

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

Fin.

4.5 HomogenisationExample: simulate heterogeneous diffusion in 1D on patches

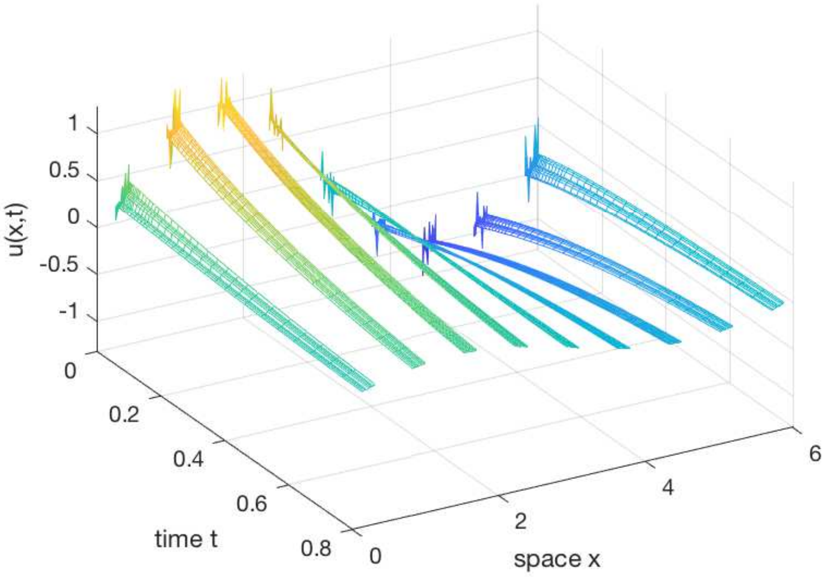
Subsection contents

Figures 14 and 15 show example simulations in time generated by the patch scheme function applied to heterogeneous diffusion. That such simulations of heterogeneous diffusion makes valid predictions was established by **?** 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. We present two different methods of obtaining a macroscale solution. One method uses the given heterogeneous diffusion, which produces a solution which has microscale roughness (Figure 14). The other method constructs an ensemble of heterogeneous diffusion and produces an ensemble average solution which has a smooth microscale (Figure 15).

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

1. configPatches1
2. ode15s $\leftrightarrow$ patchSmooth1 $\leftrightarrow$ heteroDiff

Figure 14: the diffusing field $u(x,t)$ in the patch (gap-tooth) scheme applied to microscale heterogeneous diffusion with no ensemble average. The heterogeneous diffusion results in a smilarly heterogeneous field solution.



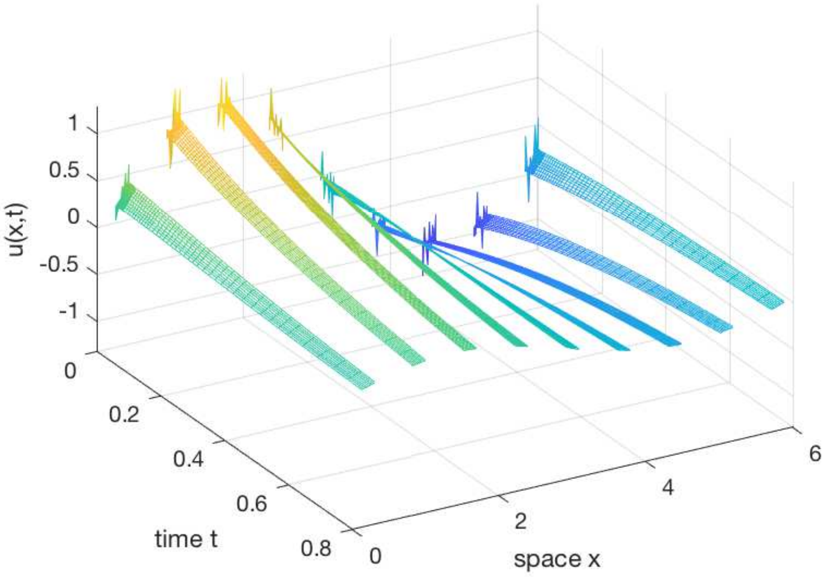
3. process results

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

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

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

Figure 15: the diffusing field $u(x,t)$ in the patch (gap-tooth) scheme applied to microscale heterogeneous diffusion with an ensemble average. The ensemble average smooths out the heterogeneous diffusion.



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).

```
clear all
mPeriod = 4
rng('default'); rng(1);
cDiff = exp(4*rand(mPeriod,1))
cHomo = 1/mean(1./cDiff)
```

Establish global data struct `patches` for heterogeneous diffusion solved on 2π-periodic domain, with nine patches, each patch of half-size 0.2. A user can add information to patches in order to communicate to the time derivative function. Quadratic (fourth-order) interpolation ordCC $= 4$ provides values for the inter-patch coupling conditions. The odd integer patches.nCore $=$ 3 defines the size of the patch core (this must be larger than zero and less than nSubP), where a core of size zero indicates that the value in the centre of the patch gives the macroscale. The introduction of a finite width core requires a redefinition of the half-patch ratio, as described by ?. The Boolean patches.Ens indicates whether or not we apply ensemble averaging of diffusivity configurations. We evaluate the patch coupling by interpolating the core.

```
global patches
nPatch = 9
ratio = 0.2
nSubP = 11
Len = 2*pi;
ordCC=4;
patches.nCore=3;
patches.ratio = ratio*(nSubP - patches.nCore)/(nSubP - 1);
patches.EnsAve=0;
configPatches1(@heteroDiff,[0 Len],nan,nPatch, ...
 ordCC,patches.ratio,nSubP);
```

A (nSubP-1) $\times$ nPatch matrix defines the diffusivity coefficients within each patch. In the case of ensemble averaging, nVars becomes the size of the ensemble (for the case of no ensemble averaging nVars is the number of different field variables, which in this example is nVars $= 1$) and we use the ensemble described by ? which includes all reflected and translated configurations of patches.cDiff. With ensemble averaging we must increase the size of the diffusivity matrix to (nSubP-1) $\times$ nPatch $\times$ nVars.

```
patches.cDiff = cDiff((mod(round(patches.x(1:(end-1),:) ...
  /(patches.x(2)-patches.x(1))-0.5),mPeriod)+1));
if patches.EnsAve
  if mPeriod>2
    nVars=2*mPeriod;
  else
    nVars=mPeriod;
  end
  patches.cDiff=repmat(patches.cDiff,[1,1,nVars]);
  for sx=2:mPeriod
    patches.cDiff(:,:,sx)=circshift( ...
      patches.cDiff(:,:,sx-1),[sx-1,0]);
   end;
   if nVars>2
     patches.cDiff(:,:,(mPeriod+1):end)=flipud( ...
       patches.cDiff(:,:,1:mPeriod));
   end;
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.

```
u0 = sin(patches.x)+0.2*randn(nSubP,nPatch);
%u0 = exp(-2*(patches.x-Len/2).^2).*(1+0.1*rand(nSubP,nPatch));
if patches.EnsAve
  u0 = repmat(u0,[1,1,nVars]);
end
[ts,ucts] = ode15s(@patchSmooth1, [0 2/cHomo], u0(:));
ucts=reshape(ucts,length(ts),length(patches.x(:)),[]);
```

Plot the simulation in Figure 14 (with no ensemble average) or Figure 15 (with an ensemble average). If we have calculated an ensemble of field solutions, then we must first take the ensemble average.

```
if patches.EnsAve % calculate the ensemble average
  uctsAve=mean(ucts,3);
else
  uctsAve=ucts;
```

```
end
figure(1),clf
xs = patches.x;  xs([1 end],:) = nan;
mesh(ts,xs(:),uctsAve'),  view(60,40)
xlabel('time t'), ylabel('space x'), zlabel('u(x,t)')
set(gcf,'PaperUnits','centimeters');
set(gcf,'PaperPosition',[0 0 14 10]);
if patches.EnsAve
  print('-depsc2','ps1HomogenisationCtsUEnsAve')
else
  print('-depsc2','ps1HomogenisationCtsU')
end
```

Use projective integration in time Now take `patchSmooth1`, the interface to the time derivatives, and wrap around it the projective integration `PIRK2` (Section 3.1), of bursts of simulation from `heteroBurst` (Section 4.5.3), as illustrated by Figures 16 and 17.

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

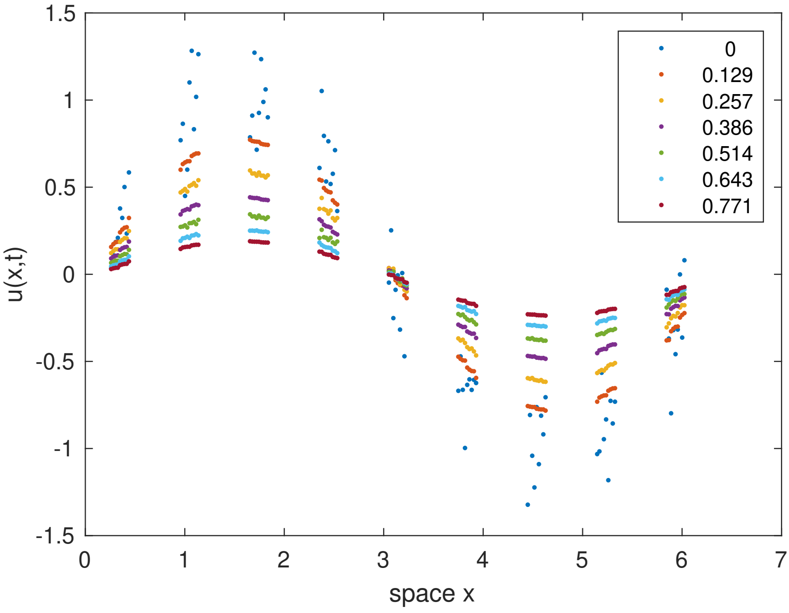
1. configPatches1 (done in first part)
2. PIRK2 ↔ heteroBurst ↔ micro-integrator ↔ patchSmooth1 ↔ heteroDiff
3. process results

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

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

Set the desired macro- and 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.

Figure 16: field $u(x,t)$ shows basic projective integration of patches of heterogeneous diffusion with no ensemble average: different colours correspond to the times in the legend. This field solution displays some fine scale heterogeneity due to the heterogeneous diffusion.

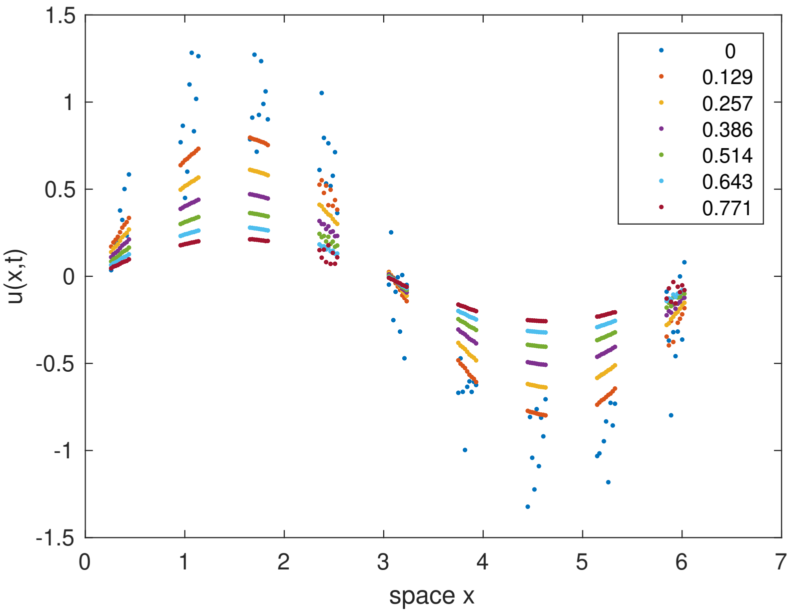


```
ts = linspace(0,2/cHomo,7)
bT = 3*( ratio*Len/nPatch )^2/cHomo
addpath('../ProjInt','../SandpitPlay/RKint')
[us,tss,uss] = PIRK2(@heteroBurst, bT, ts, u0(:));
```

Plot the macroscale predictions to draw Figure 16 or Figure 17. If we have calculated an ensemble of field solutions, then we must first take the ensemble average.

```
if patches.EnsAve % calculate the ensemble average
  usAve=mean(reshape(us,size(us,1),length(xs(:)),nVars),3);
  ussAve=mean(reshape(uss,length(tss),length(xs(:)),nVars),3);
else
```

Figure 17: field $u(x,t)$ shows basic projective integration of patches of heterogeneous diffusion with ensemble average: different colours correspond to the times in the legend. Once transients have decayed, this field solution is smooth due to the ensemble average.



```
  usAve=us;
  ussAve=uss;
end
figure(2),clf
plot(xs(:),usAve','.')
ylabel('u(x,t)'), xlabel('space x')
legend(num2str(ts',3))
set(gcf,'PaperUnits','centimeters');
set(gcf,'PaperPosition',[0 0 14 10]);
if patches.EnsAve
  print('-depsc2','ps1HomogenisationUEnsAve')
else
```

Figure 18: stereo pair of the field $u(x, t)$ during each of the microscale bursts used in the projective integration with no ensemble averaging.

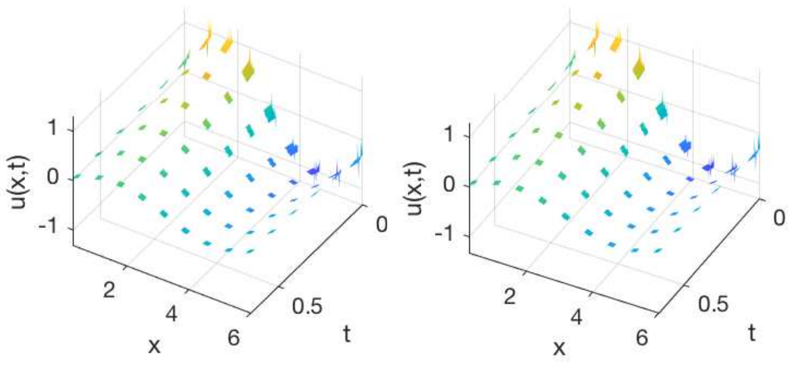
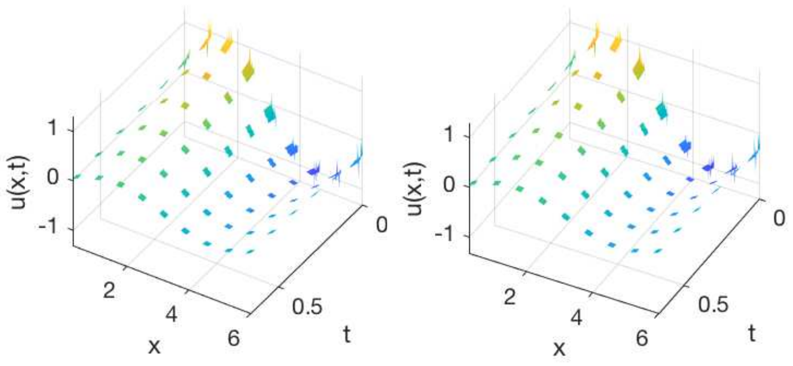


Figure 19: stereo pair of the field $u(x, t)$ during each of the microscale bursts used in the projective integration with ensemble averaging.



```
  print('-depsc2','ps1HomogenisationU')
end
```

Also plot a surface detailing the microscale bursts as shown in Figure 18 or Figure 19.

```
figure(3),clf
```

```
for k = 1:2, subplot(1,2,k)
  surf(tss,xs(:),ussAve',  'EdgeColor','none')
  ylabel('x'), xlabel('t'), zlabel('u(x,t)')
  axis tight, view(126-4*k,45)
end
set(gcf,'PaperUnits','centimeters');
set(gcf,'PaperPosition',[0 0 14 6]);
if patches.EnsAve
  print('-depsc2','ps1HomogenisationMicroEnsAve')
else
  print('-depsc2','ps1HomogenisationMicro')
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.

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

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 four possibilities:

- ode23 generates 'noise' that is unsightly at best and may be ruinous;
- ode45 is similar to ode23, but with reduced noise;
- ode15s does not cater for the NaNs in some components of u;
- rk2int simple specified step integrator, but may require inefficiently small time steps.

```
function [ts, ucts] = heteroBurst(ti, ui, bT)
  switch '45'
  case '23',  [ts,ucts] = ode23(@patchSmooth1,[ti ti+bT],ui(:));
  case '45',  [ts,ucts] = ode45(@patchSmooth1,[ti ti+bT],ui(:));
  case '15s', [ts,ucts] = ode15s(@patchSmooth1,[ti ti+bT],ui(:));
  case 'rk2', ts = linspace(ti,ti+bT,200)';
              ucts = rk2int(@patchSmooth1,ts,ui(:));
  end
end
```

Fin.

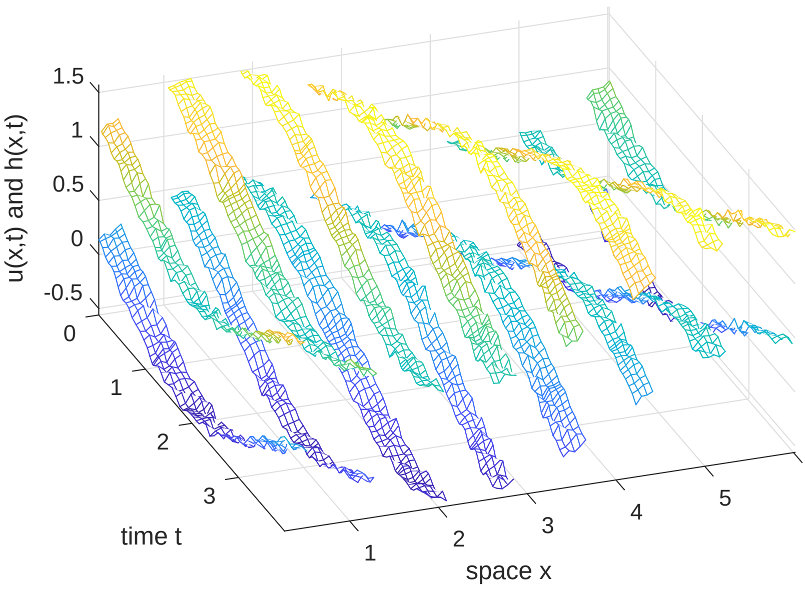
4.6 waterWaveExample: simulate a water wave PDE on patches

Subsection contents

Figure 20 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

Figure 20: 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.



microscale simulator of the nonlinear shallow water wave PDE derived from the Smagorinski model of turbulent flow (**??**).

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

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

where the brackets indicate that the nonlinear functions f_ℓ may involve various spatial derivatives of the fields $h(x,t)$ and $u(x,t)$. For example, Section 4.6.3 encodes a nonlinear Smagorinski model of turbulent shallow water (**??**, 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

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

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

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 $h|u|\partial^2u/\partial x^2$, and gravitational hydrostatic forcing $\tan\theta - \partial h/\partial x$. Figure 21 shows one simulation of this system—for the same initial condition as Figure 20.

For such wave systems, let's implement a staggered microscale grid and staggered macroscale patches as introduced by **?** in their Figures 3 and 4, respectively.

4.6.1 Script code to simulate wave systems

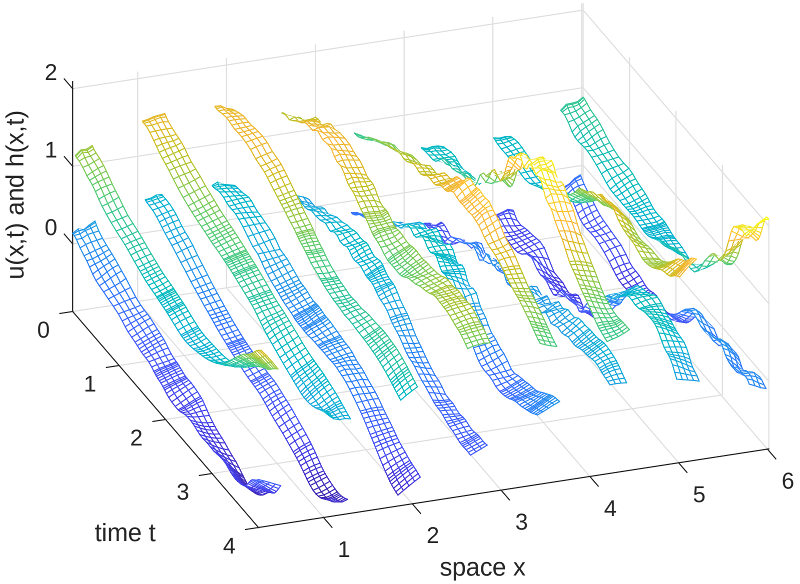
This script implements the following gap-tooth scheme (arrows indicate function recursion).

1. configPatches1, and add micro-information
2. ode15s ↔ patchSmooth1 ↔ simpleWavePDE
3. process results
4. ode15s ↔ patchSmooth1 ↔ waterWavePDE
5. process results

Establish the global data struct `paches` for the PDEs (2) (linearised) solved on 2π-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).

```
clear all
global patches
```

Figure 21: 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.



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

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

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

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

```
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.

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

Plot the simulation.

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

Print the output.

```
  set(gcf,'paperposition',[0 0 14 10])
  if k==1, print('-depsc2','ps1WaveCtsUH')
  else print('-depsc2','ps1WaterWaveCtsUH')
  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.

```
  patches.fun = @waterWavePDE;
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.

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

Compute the PDE derivatives at interior points of the patches.

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

Here 'wastefully' compute time derivatives for both PDEs at all grid points—for 'simplicity'—and then 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.

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

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

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

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

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

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()`.

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

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

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

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

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

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

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

Correspondingly estimate the terms in the momentum PDE: u-values in $\texttt{U}_i$ and $\texttt{V}_{i\pm1}$; and h-values in $\texttt{V}_i$ and $\texttt{U}_{i\pm1}$.

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

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

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

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

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

Fin.

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

Subsubsection contents

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

```
function configPatches2(fun,Xlim,BCs,nPatch,ordCC,ratio,nSubP,nEdge)
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 **??** 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)`] × [`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` $= \frac{1}{2}$ 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)` $\times$ `nPatch(1)` array of the regular spatial locations x_{ij} of the microscale grid points in every patch.
- `.y` is `nSubP(2)` $\times$ `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.

4.8 `patchSmooth2()`: interface to time integrators

Subsubsection contents

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`.

```
function dudt=patchSmooth2(t,u)
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.

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

Subsubsection contents

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.

```
function u=patchEdgeInt2(u)
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` $\times$ `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` $\times$ `ny` $\times$ `Nx` $\times$ `Ny` $\times$ `nVars` array of the fields with edge values set by interpolation.

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

Subsection contents

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

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

This script shows one way to get started: a user's script may have the following three steps (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 2π-periodic domain, with 9×9 patches, spectral interpolation couples the patches, each patch of half-size ratio 0.25, and with 5×5 points within each patch.

```
clear all, close all
global patches
nSubP = 5;
nPatch = 9;
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.

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

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

```
small=1;
jac=nan(length(i));
sizejac=size(jac)
for j=1:length(i)
  uv=uv0(:);
  uv(i(j))=uv(i(j))+small;
  tmp=patchSmooth2(0,uv)/small;
  jac(:,j)=tmp(i);
end
```

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

```
evals=eig(jac);
nEvals=length(evals)
[~,k]=sort(-abs(real(evals)));
evalsWithBiggestRealPart=evals(k(1:10))
if abs(real(evals(k(1))))>1e-4
```

```
    warning('eigenvalue failure: real-part > 1e-4')
    return, end
```

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

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

4.10.2 Execute a simulation

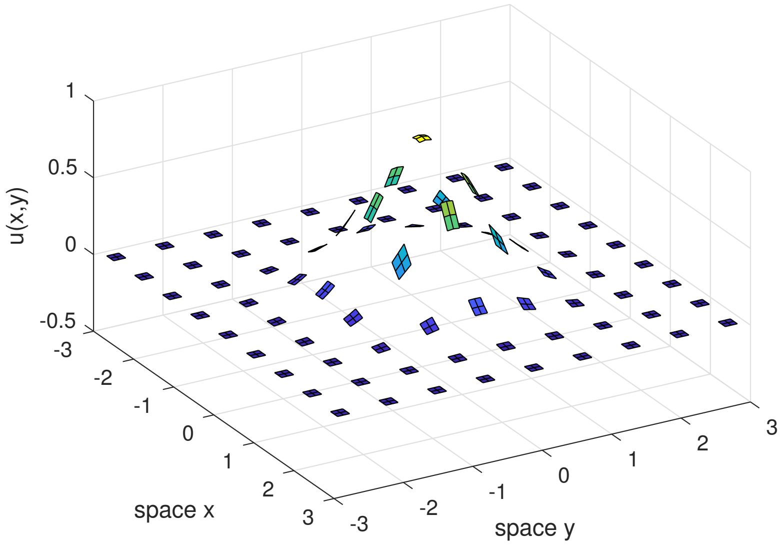
Set a Gaussian initial condition using auto-replication of the spatial grid: here u0 and v0 are in the form required for computation: $n_x \times n_y \times N_x \times N_y$.

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

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

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

Figure 22: initial field $u(x, y, t)$ at time $t = 0$ of the patch scheme applied to the simple wave PDE: Figure 23 plots the computed field at time $t = 6$.



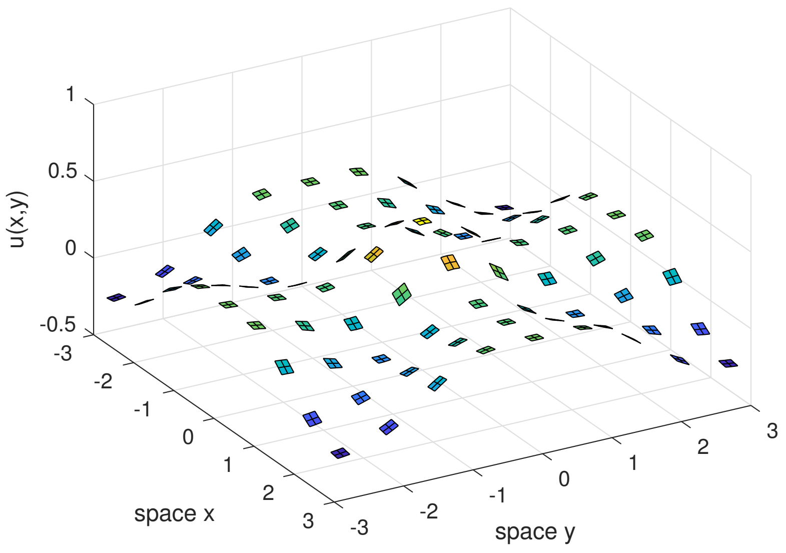
Integrate in time using standard functions.

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

Animate the computed simulation to end with Figure 23. Subsample to plot at most 200 times.

```
di = ceil(length(ts)/200);
for i = [1:di:length(ts)-1 length(ts)]
  uv = patchEdgeInt2(uvs(i,:));
  uv = reshape(permute(uv,[1 3 2 4 5]), [numel(x) numel(y) 2]);
  usurf.ZData = uv(:,:,1)';
  title(['wave PDE on patches: time = ' num2str(ts(i))])
  pause(0.1)
end
title('')
```

Figure 23: field $u(x, y, t)$ at time $t = 6$ of the patch scheme applied to the simple wave PDE with initial condition in Figure 22.



```
set(gcf,'paperposition',[0 0 14 10])
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 $\dot v_{ijkl} = \frac{1}{\delta x^2}(u_{i+1,j,k,l} - 2u_{i,j,k,l} + u_{i-1,j,k,l}) + \frac{1}{\delta y^2}(u_{i,j+1,k,l} - 2u_{i,j,k,l} + u_{i,j-1,k,l})$.

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

```
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

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

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

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

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

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

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

```
for k=1:nPatch/2
  u0=sin(k*patches.x*2*pi/Len);
  v0=cos(k*patches.x*2*pi/Len);
  uvi=patchEdgeInt1([u0(:);v0(:)]);
  normuError=norm(uvi(:,:,1)-u0)*norm(u0(i0,:));
  normvError=norm(uvi(:,:,2)-v0)*norm(v0(i0,:));
  if abs(normuError)+abs(normvError)>2e-13
    normuError=normuError, normvError=normvError
    error(['failed double field interpolation k=' num2str(k)])
  end
end
```

End the for-loop over various geometries.

```
end
```

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

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

Identify which microscale grid points are h or u values.

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

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

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

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

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

End for-loop over patches

```
end
```

Finish If no error messages, then all OK.

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

4.13 `patchEdgeInt2test`: tests 2D spectral interpolation

Try 99 realisations of random tests.

```
clear all, close all
global patches
for realisation=1:99
```

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

```
Lx=1+3*rand, Ly=1+3*rand
nSubP=1+2*randi(3,1,2)
ratios=rand(1,2)/2
nPatch=2+randi(4,1,2)
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.

```
nV=randi(3)
[nx,Nx]=size(patches.x);
[ny,Ny]=size(patches.y);
u0s=nan(nx,ny,Nx,Ny,nV);
for iV=1:nV
  kx=randi([0 ceil((nPatch(1)-1)/2)])
  ky=randi([0 ceil((nPatch(2)-1)/2)])
  phix=pi*rand*(2*kx~=nPatch(1))
  phiy=pi*rand*(2*ky~=nPatch(2))
  % generate 2D array via auto-replication
  u0=sin(2*pi*kx*patches.x(:) /Lx+phix) ...
   .*sin(2*pi*ky*patches.y(:)'/Ly+phiy);
  % reshape into 4D array
  u0=reshape(u0,[nx Nx ny Ny]);
  u0=permute(u0,[1 3 2 4]);
  % store into 5D array
  u0s(:,:,:,:,iV)=u0;
end
```

Copy and NaN the edges, then interpolate

```
u=u0s; u([1 end],:,:,:,:)=nan; u(:,[1 end],:,:,:)=nan;
```

```
u=patchEdgeInt2(u(:));
```

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

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

References

Gear, C. W., Kaper, T. J., Kevrekidis, I. G. & Zagaris, A. (2005), 'Projecting to a slow manifold: Singularly perturbed systems and legacy codes', *SIAM Journal on Applied Dynamical Systems* **4**(3), 711–732.

Gear, C. W. & Kevrekidis, I. G. (2003*a*), 'Projective methods for stiff differential equations: Problems with gaps in their eigenvalue spectrum', *SIAM Journal on Scientific Computing* **24**(4), 1091–1106.
http://link.aip.org/link/?SCE/24/1091/1

Gear, C. W. & Kevrekidis, I. G. (2003*b*), 'Telescopic projective methods for parabolic differential equations', *Journal of Computational Physics* **187**, 95–109.

Givon, D., Kevrekidis, I. G. & Kupferman, R. (2006), 'Strong convergence of projective integration schemes for singularly perturbed stochastic differential systems', *Comm. Math. Sci.* **4**(4), 707–729.

Hyman, J. M. (2005), 'Patch dynamics for multiscale problems', *Computing in Science & Engineering* **7**(3), 47–53.
http://scitation.aip.org/content/aip/journal/cise/7/3/10.1109/MCSE.2005.57

Kevrekidis, I. G., Gear, C. W. & Hummer, G. (2004), 'Equation-free: the computer-assisted analysis of complex, multiscale systems', *A. I. Ch. E. Journal* **50**, 1346–1354.

Kevrekidis, I. G., Gear, C. W., Hyman, J. M., Kevrekidis, P. G., Runborg, O. & Theodoropoulos, K. (2003), 'Equation-free, coarse-grained multiscale computation: enabling microscopic simulators to perform system level tasks', *Comm. Math. Sciences* **1**, 715–762.

Kevrekidis, I. G. & Samaey, G. (2009), 'Equation-free multiscale computation: Algorithms and applications', *Annu. Rev. Phys. Chem.* **60**, 321—44.

Liu, P., Samaey, G., Gear, C. W. & Kevrekidis, I. G. (2015), 'On the acceleration of spatially distributed agent-based computations: A patch dynamics scheme', *Applied Numerical Mathematics* **92**, 54–69.

http://www.sciencedirect.com/science/article/pii/S0168927414002086

Roberts, A. J. & Kevrekidis, I. G. (2007), ‘General tooth boundary conditions for equation free modelling’, *SIAM J. Scientific Computing* **29**(4), 1495–1510.

Samaey, G., Kevrekidis, I. G. & Roose, D. (2005), ‘The gap-tooth scheme for homogenization problems’, *Multiscale Modeling and Simulation* **4**, 278–306.

Samaey, G., Roose, D. & Kevrekidis, I. G. (2006), ‘Patch dynamics with buffers for homogenization problems’, *J. Comput Phys.* **213**, 264–287.

Zagaris, A., Vandekerckhove, C., Gear, C. W., Kaper, T. J. & Kevrekidis, I. G. (2012), ‘Stability and stabilization of the constrained runs schemes for equation-free projection to a slow manifold’, *DCDS-A* **32**, 2759–2803.