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

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Abstract

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

1 Introduction

Users Place this toolbox's folder in a path searched by MATLAB/Octave. Then read the section 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

Chapter 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 Chapter 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. Chapter 3 fully details each function.

The cheat sheet consists of two flow charts. Figure 2.1 overviews constructing a PI simulation. Figure 2.2 roughly guides which of the top-level PI functions should be used.

2.2 Cheat sheet: constructing patches

This section pertains to the Patch approach, Chapter 4, to solving PDEs, lattice systems, or agent/particle microscale simulators.

The Patch toolbox requires that one configure patches, couple the patches and interface the coupled patches with a time integrator. Figure 2.3 overviews the chief functions involved and their interactions.

Figure 2.1: these figures appear confusing to a newbie???? and we must not *resize fixed width constructs. Use linewidth for large-scale layout scaling, em for small-widths, and ex for small-heights.*

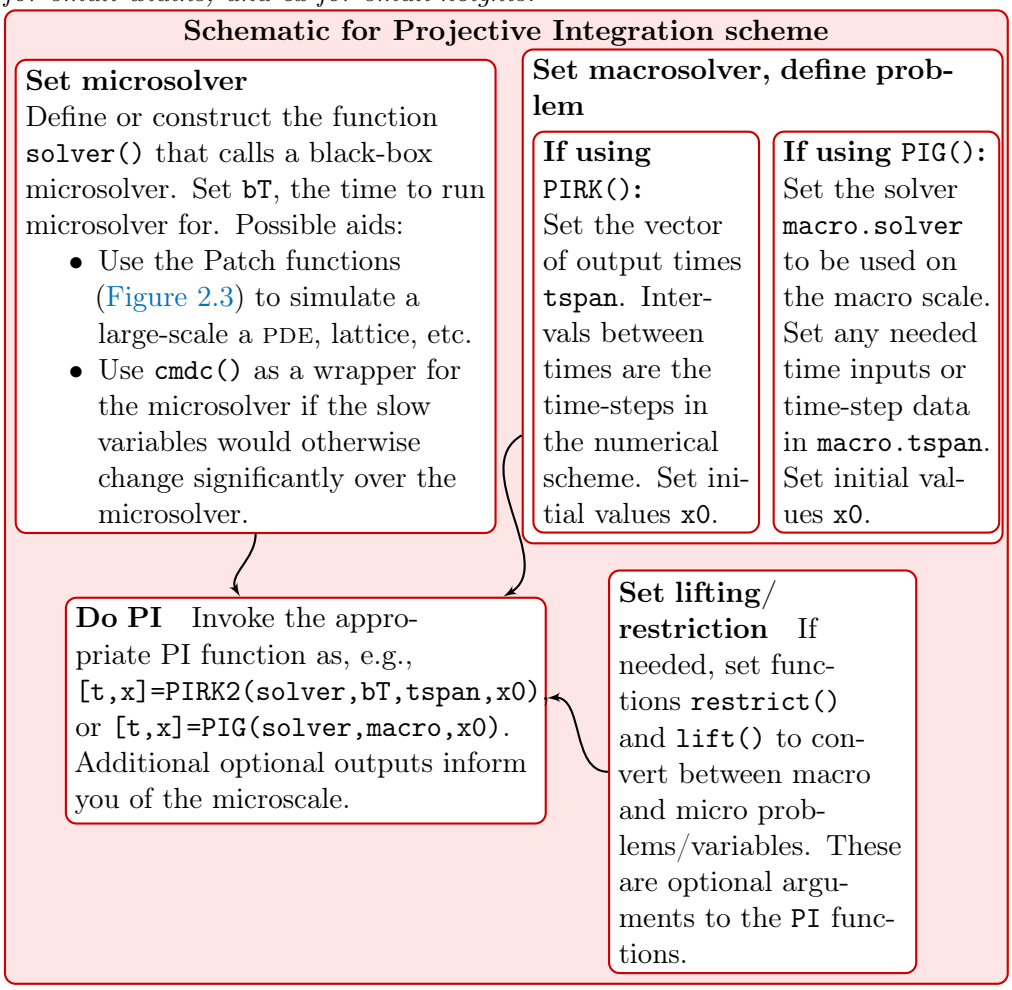


Figure 2.2:

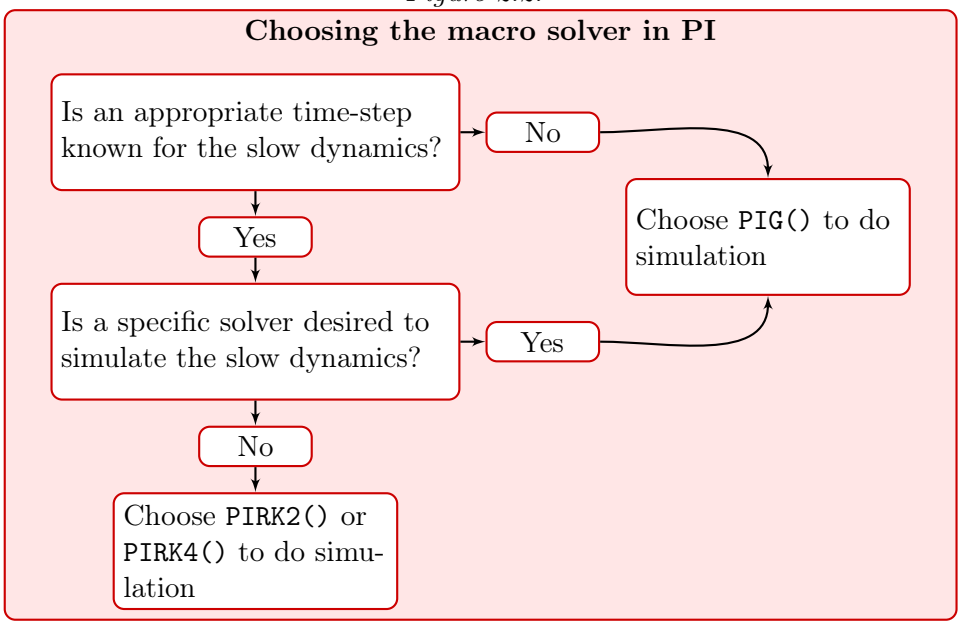
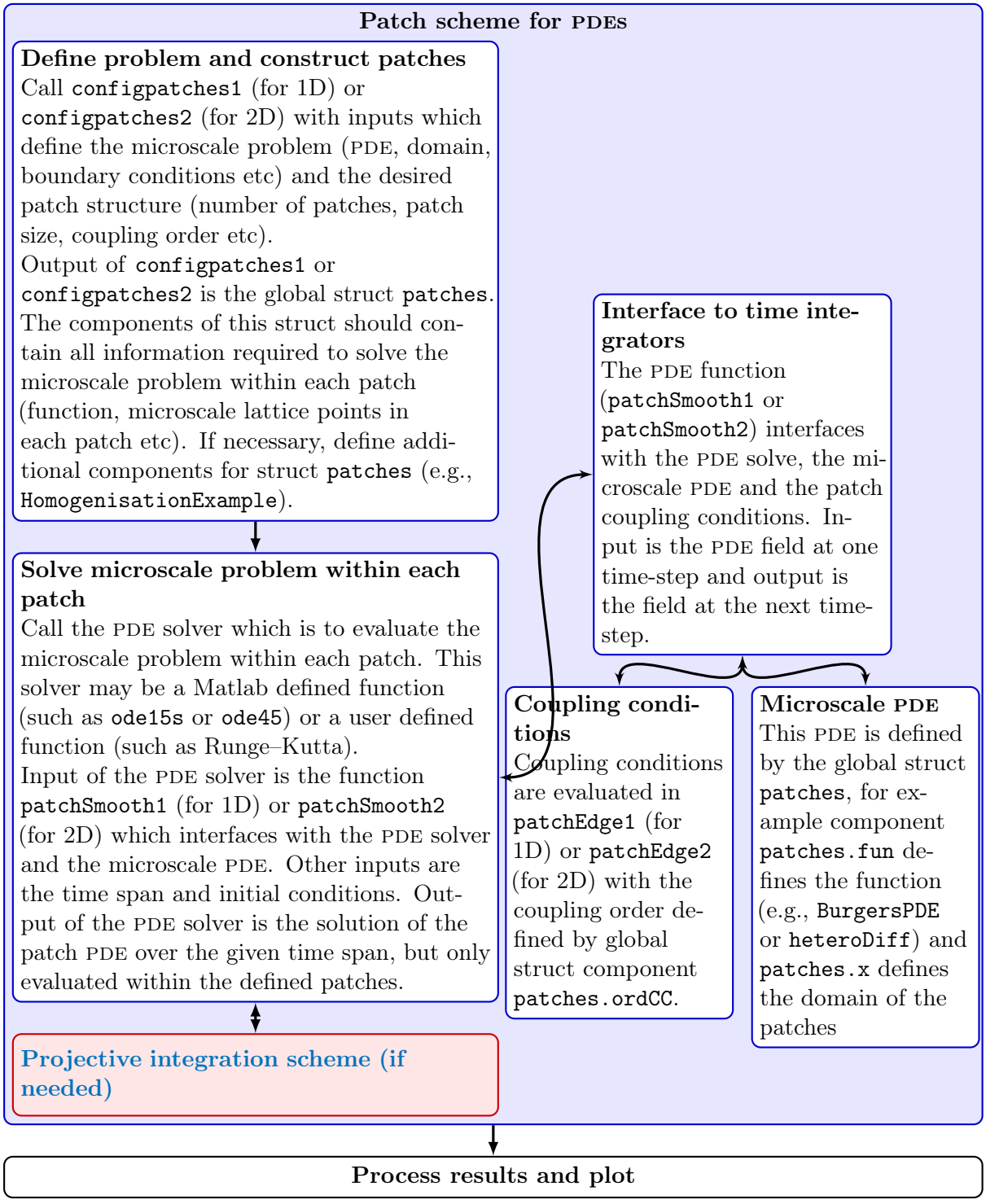

Choosing the macro solver in PI
Is an appropriate time-step known for the slow dynamics?
No
Choose PIG() to do simulation
Yes
Is a specific solver desired to simulate the slow dynamics?
Yes
No
Choose PIRK2() or PIRK4() to do simulation

Figure 2.3:


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, define additional components for struct patches (e.g., 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.
Projective integration scheme (if needed)
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
Process results and plot

3 Projective integration of deterministic ODEs

Chapter contents

3.1 Introduction

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 3.3 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()`.

3.2 `PIRK2()`: projective integration of second-order accuracy

Section contents

3.2.1 Introduction

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

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

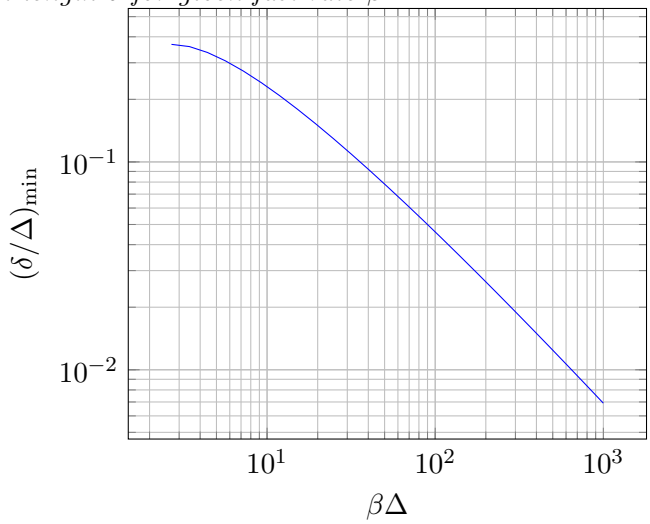
Input If there are no input arguments, then this function applies itself to the Michaelis–Menton example: see the code in Section 3.2.2 as a basic template of how to use.

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

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

  – Inputs: `tStart`, the start time of a burst of simulation; `xStart`, the row n-vector of the starting state; `bT`, optional, the total time to simulate in the burst—if `microBurst()` determines the burst time, then replace `bT` in the argument list by `varargin`.

Figure 3.1: 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.



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

- `tSpan` is an ℓ-vector of times at which the user requests output, of which the first element is always the initial time. `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.
- `bT`, optional, either missing, or empty (`[]`), or a scalar: if a given scalar, then it is the length of the micro-burst simulations—the minimum amount of time needed for the microscale simulation to relax to the slow manifold; else if missing or `[]`, then `microBurst()` must itself determine the length of a computed burst.

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

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 3.1).

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

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

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

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

- `xms`, optional, is an $L \times n$ array of the corresponding microscale states—this data is an accurate simulation of the state and may help visualise more details of the solution.

- `rm`, optional, a struct containing the 'remaining' applications of the 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.

3.2.2 If no arguments, then execute an example

```
174 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, ts, [1;0], bT);
figure, plot(ts,x,'o:',tms,xms)
title('Projective integration of Michaelis--Menten enzyme kinetics')
xlabel('time t'), legend('x(t)','y(t)')
```

Upon finishing execution of the example, exit this function.

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

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
```

3.3 egPIMM: Example projective integration of Michaelis–Menton kinetics

Section contents

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

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

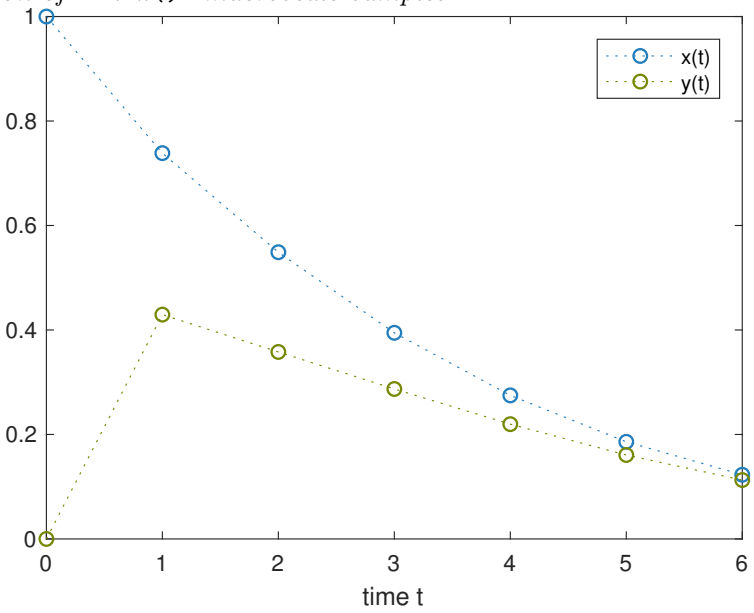
As illustrated in Figure 3.3, the slow variable $x(t)$ evolves on a time scale of one, whereas the fast variable $y(t)$ evolves on a time scale of the small parameter ϵ.

3.3.1 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
```

Figure 3.2: Michaelis–Menten enzyme kinetics simulated with the projective integration of `PIRK2()`: macroscale samples.



First, Section 3.3.2 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, ts, [1;0], 2*epsilon)
plot(ts,xs,'o:')
xlabel('time t'), legend('x(t)','y(t)')
pause(1)
```

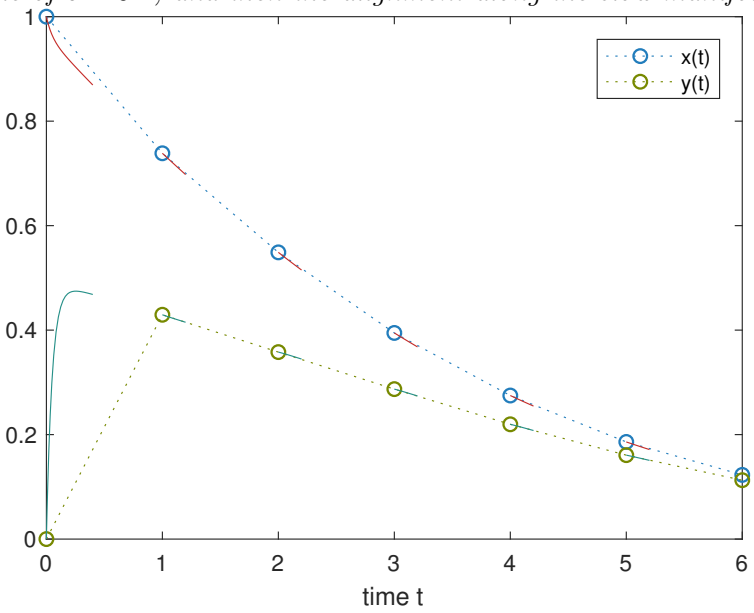
Figure 3.2 plots the macroscale results showing the long time decay of the Michaelis–Menten system on the slow manifold. **?** [§4] used this system as an example of their analysis of the convergence of Projective Integration.

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 3.2). To see the initial transient attraction to the slow manifold we plot some microscale data in Figure 3.3. Two further output variables provide this microscale burst information.

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

Figure 3.3 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

Figure 3.3: 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.*



also affected by the initial transient which indicates that other schemes which 'freeze' slow variables are less accurate.

Optional: simulate backwards in time Figure 3.4 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.

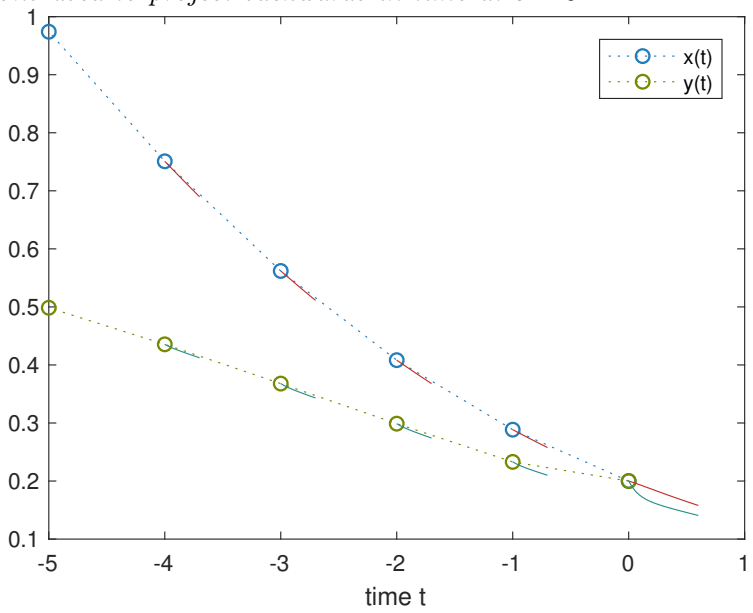
```
111 ts = 0:-1:-5
112 [xs,tMicro,xMicro] = PIRK2(@MMburst, ts, 0.2*[1;1], 3*epsilon);
113 figure, plot(ts,xs,'o:',tMicro,xMicro)
114 xlabel('time t'), legend('x(t)','y(t)')
```

3.3.2 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.

```
141 function [ts, xs] = MMburst(ti, xi, bT)
142     global epsilon
143     dMMdt = @(t,x) [ -x(1)+(x(1)+0.5)*x(2)
144           1/epsilon*( x(1)-(x(1)+1)*x(2) ) ];
145     [ts, xs] = ode23(dMMdt, [ti ti+bT], xi);
146 end
```

Figure 3.4: 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 $\epsilon = 0.1$.



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

Section contents

3.4.1 Introduction

This is a Projective Integration scheme when the macroscale integrator is any specified 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 integration/simulation.

By default, `PIG()` uses 'constraint-defined manifold computing' for the microscale simulations. This algorithm, initiated by `?`, uses a backwards projection so that the simulation time is unchanged after running the microscale simulator. The implementation is `cdmc()`, described in Section 3.5.2.

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

Inputs:

- `macroInt()`, the numerical method that the user wants to apply on a slow-time macroscale. Either input a standard MATLAB/Octave integration function (such as `'ode23'` or `'ode45'`), or code your own

integration function using standard arguments. That is, if you code your own, then it must be

```
[Ts,Xs] = macroInt(F,Tspan,X0)
```

where

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- `T`, an L-vector of times at which `macroInt` produced results.
- `X`, an $L \times N$ array of the computed solution: the ith *row* of `X`, `X(i,:)`, is to be the macro-state vector $\vec{X}(t)$ at time $t =$ `T(i)`.

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

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

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

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

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

3.4.2 If no arguments, then execute an example

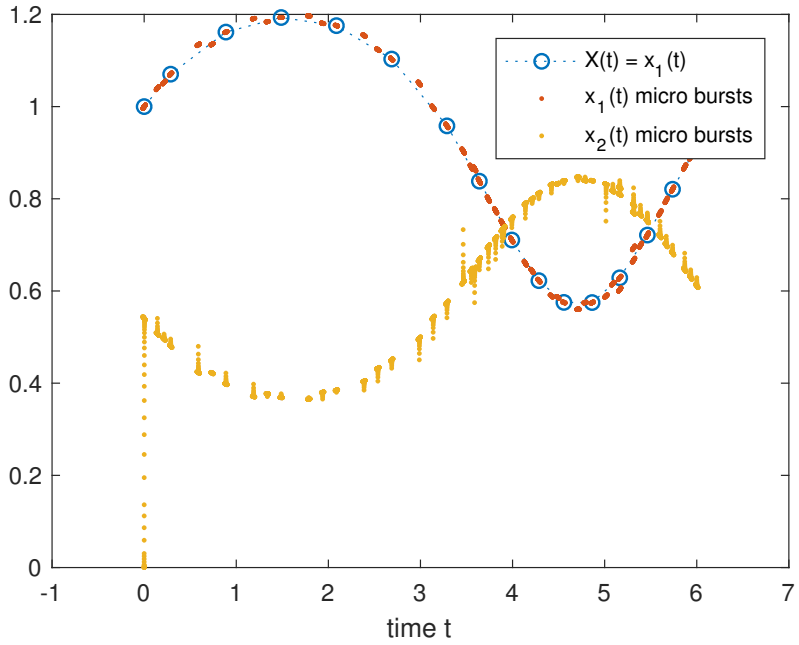
```
179 if nargin==0
```

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

$$\frac{dx_1}{dt} = \cos(x_1)\sin(x_2)\cos(t) \quad \text{and} \quad \frac{dx_2}{dt} = \frac{1}{\epsilon}\big[\cos(x_1) - x_2\big]. \tag{3.1}$$

The macroscale variable is $X(t) = x_1(t)$, and the evolution dX/dt is unclear. With initial condition $X(0) = 1$, the following code computes and

Figure 3.5: Projective Integration by `PIG` *of the example system (3.1) in Section 3.4.2. The macroscale solution $X(t)$ is represented by just the blue circles. The microscale bursts are the microscale states $(x_1(t), x_2(t)) = (red, yellow)$ dots.*



plots a solution of the system (3.1) over time $0 \le t \le 6$ for parameter $\epsilon = 10^{-3}$(Figure 3.5). Whenever needed by `microBurst()`, the microscale system (3.1) is initialised ('`lift`ed') using $x_2(t) = x_2^{\text{approx}}$ (yellow dots in Figure 3.5).

First we code the right-hand side function of the microscale system (3.1) of ODEs.

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

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

```
bT = 2*epsilon*log(1/epsilon)
microBurst = @(tb0,xb0) ode45(dxdt,[tb0 tb0+bT],xb0);
```

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

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

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

```
247 Tspan = [0 6];
248 x0 = [1;0];
249 [Ts,Xs,tms,xms] = PIG('ode23',microBurst,Tspan,x0,restrict,lift);
```

Plot output of this projective integration.

```
255 figure, plot(Ts,Xs,'o:',tms,xms,'.')
256 title('Projective integration of singularly perturbed ODE')
257 xlabel('time t')
258 legend('X(t) = x_1(t)','x_1(t) micro bursts','x_2(t) micro bursts')
```

Upon finishing execution of the example, exit this function.

```
264 return
265 end%if no arguments
```

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

Section contents

3.5.1 Introduction

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

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

See Section 3.2 as the inputs and outputs are the same as PIRK2().

If no arguments, then execute an example

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

Example of Michaelis–Menton backwards in time The Michaelis–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 $-5 \le t \le 0$ 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, ts, 0.2*[1;1], bT);
figure, plot(ts,x,'o:',tms,xms)
xlabel('time t'), legend('x(t)','y(t)')
title('Backwards-time projective integration of Michaelis--Menten')
```

Upon finishing execution of the example, exit this function.

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

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
```

3.5.2 `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.

4 Patch scheme for given microscale discrete space system

Chapter contents

4.1 Introduction

The patch scheme applies to spatio-temporal systems where the spatial domain is larger than what can be computed in reasonable time. In the scheme we compute 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 See Sections 4.2.2 and 4.5.2 which list example basic code that uses the provided functions to simulate 1D Burgers' PDE and a 2D nonlinear 'diffusion' PDE.

4.2 `configPatches1()`: configures spatial patches in 1D

Section contents

4.2.1 Introduction

Makes the struct `patches` for use by the patch/gap-tooth time derivative function `patchSmooth1()`. Section 4.2.2 lists an example of its use.

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

Input If invoked with no input arguments, then executes an example of simulating Burgers' PDE—see Section 4.2.2 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 ≥ -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`, optional, 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.

4.2.2 If no arguments, then execute an example

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

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

1. configPatches1
2. ode15s integrator ↔ patchSmooth1 ↔ user's burgersPDE
3. process results

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

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

Set an initial condition, with some randomness, and simulate in time using a standard stiff integrator and the interface function `patchsmooth1()` (Section 4.3).

```
128 u0=0.3*(1+sin(patches.x))+0.1*randn(size(patches.x));
129 [ts,ucts]=ode15s(@patchSmooth1,[0 0.5],u0(:));
```

Plot the simulation using only the microscale values interior to the patches: set x-edges to `nan` to leave the gaps. Figure 4.1 illustrates an example simulation in time generated by the patch scheme applied to Burgers' PDE.

```
139 figure(1),clf
140 patches.x([1 end],:)=nan;
141 surf(ts,patches.x(:),ucts'), view(60,40)
142 title('Example of Burgers PDE on patches in space')
143 xlabel('time t'), ylabel('space x'), zlabel('u(x,t)')
```

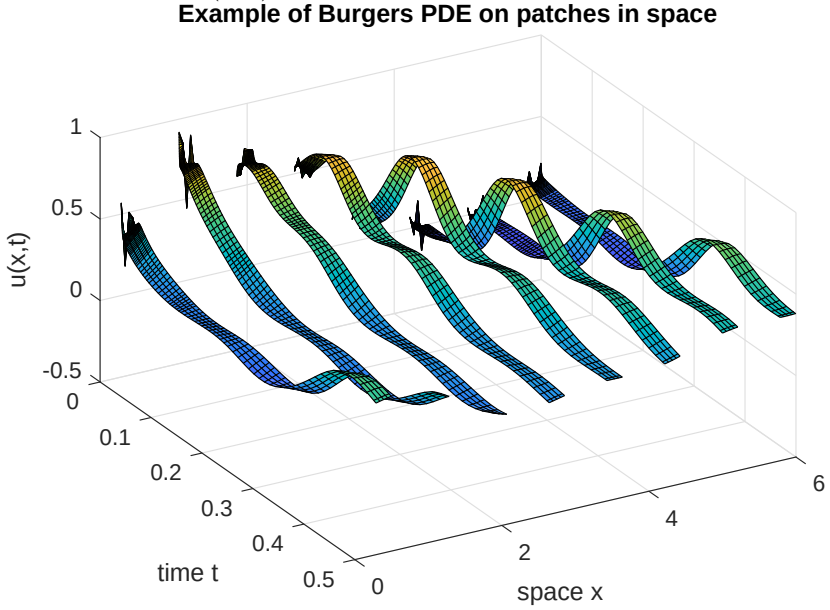
Upon finishing execution of the example, exit this function.

```
154 return
155 end%if no arguments
```

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

```
165 function ut=BurgersPDE(t,u,x)
166   dx=diff(x(1:2));  % microscale spacing
167   i=2:size(u,1)-1;  % interior points in patches
168   ut=nan(size(u));  % preallocate storage
169   ut(i,:)=diff(u,2)/dx^2 ...
170     -30*u(i,:).*(u(i+1,:)-u(i-1,:))/(2*dx);
171 end
```

Figure 4.1: field $u(x,t)$ of the patch scheme applied to Burgers' PDE.



4.3 `patchSmooth1()`: interface to time integrators

Section contents

4.3.1 Introduction

To simulate in time with spatial patches we often need to interface a user's 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` (Section 4.2).

```
25 function dudt=patchSmooth1(t,u)
26 global patches
```

Input

- `u` is a vector of length $\texttt{nSubP} \cdot \texttt{nPatch} \cdot \texttt{nVars}$ where there are `nVars` field values at each of the points in the $\texttt{nSubP} \times \texttt{nPatch}$ 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, although 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 microscales.

Output

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

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

Section contents

4.4.1 Introduction

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

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

Input

- u is a vector of length nSubP · nPatch · nVars where there are nVars field values at each of the points in the nSubP × nPatch grid.
- patches a struct set by configPatches1() which includes the following.
  - .x is nSubP × nPatch array of the spatial locations x_{ij} of the microscale grid points in every patch. Currently it *must* be an equi-spaced lattice on both macro- and microscales.
  - .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` × `nPatch` × `nVars` 2/3D array of the fields with edge values set by interpolation of patch core averages.

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

Section contents

4.5.1 Introduction

Makes the struct `patches` for use by the patch/gap-tooth time derivative function `patchSmooth2()`. Section 4.5.2 lists an example of its use.

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

Input If invoked with no input arguments, then executes an example of simulating a nonlinear diffusion PDE relevant to the lubrication flow of a thin layer of fluid—see Section 4.5.2 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 distributed equi-spaced over the interior of the rectangle $[\texttt{Xlim(1)}, \texttt{Xlim(2)}] \times [\texttt{Xlim(3)}, \texttt{Xlim(4)}]$: if `Xlim` is of length two, then use the same interval in both directions.
- `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.

4.5.2 If no arguments, then execute an example

```
123 if nargin==0
```

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

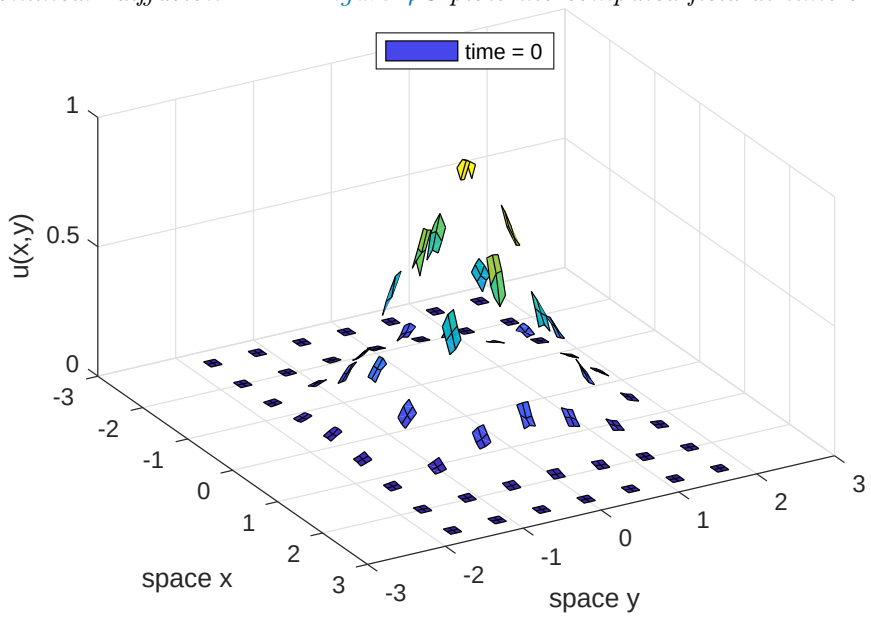
1. configPatches2
2. ode15s integrator $\leftrightarrow$ patchSmooth2 $\leftrightarrow$ user's nonDiffPDE
3. process results

Establish global patch data struct to interface with a function coding a nonlinear 'diffusion' PDE: to be solved on 6×4-periodic domain, with 9×7 patches, spectral interpolation (0) couples the patches, each patch of half-size ratio 0.25, and with 5×5 points within each patch.

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

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

Figure 4.2: initial field $u(x,y,t)$ at time $t=0$ of the patch scheme applied to a nonlinear 'diffusion' PDE: Figure 4.3 plots the computed field at time $t=3$.




```
151 x = reshape(patches.x,nSubP,1,[],1);
152 y = reshape(patches.y,1,nSubP,1,[]);
153 u0 = exp(-x.^2-y.^2);
154 u0 = u0.*(0.9+0.1*rand(size(u0)));
```

Initiate a plot of the simulation using only the microscale values interior to the patches: set x and y-edges to `nan` to leave the gaps.

```
162 figure(1), clf
163 x = patches.x; y = patches.y;
164 x([1 end],:) = nan; y([1 end],:) = nan;
```

Start by showing the initial conditions of Figure 4.2 while the simulation computes.

```
171 u = reshape(permute(u0,[1 3 2 4]), [numel(x) numel(y)]);
172 hsurf = surf(x(:),y(:),u');
173 axis([-3 3 -3 3 -0.001 1]), view(60,40)
174 legend('time = 0','Location','north')
175 xlabel('space x'), ylabel('space y'), zlabel('u(x,y)')
176 drawnow
```

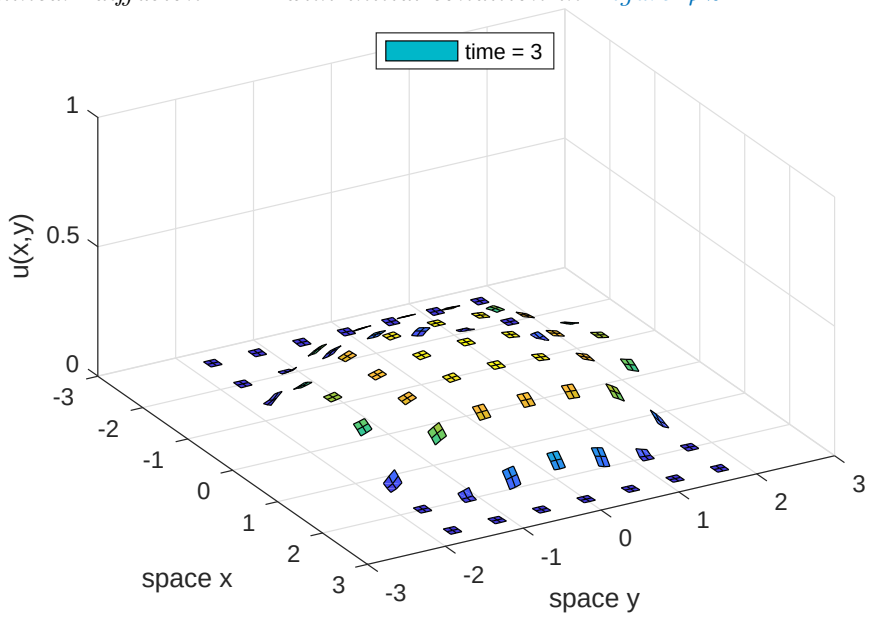
Save the initial condition to file for Figure 4.2.

```
182 set(gcf,'PaperPosition',[0 0 14 10])
183 print('-depsc2','configPatches2ic')
```

Integrate in time using standard functions.

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

Figure 4.3: field $u(x,y,t)$ at time $t = 3$ of the patch scheme applied to a nonlinear 'diffusion' PDE with initial condition in Figure 4.2.



Animate the computed simulation to end with Figure 4.3.

```
for i = 1:length(ts)
  u = patchEdgeInt2(ucts(i,:));
  u = reshape(permute(u,[1 3 2 4]), [numel(x) numel(y)]);
  hsurf.ZData = u';
  legend(['time = ' num2str(ts(i),2)])
  pause(0.1)
end
print('-depsc2','configPatches2t3')
```

Upon finishing execution of the example, exit this function.

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

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

```
function ut = nonDiffPDE(t,u,x,y)
  dx = diff(x(1:2));  dy = diff(y(1:2));  % microscale spacing
  i = 2:size(u,1)-1;  j = 2:size(u,2)-1;  % interior points in patches
  ut = nan(size(u));  % preallocate storage
  ut(i,j,:,:) = diff(u(:,j,:,:).^3,2,1)/dx^2 ...
                +diff(u(i,:,:,:).^3,2,2)/dy^2;
end
```

4.6 `patchSmooth2()`: interface to time integrators

Section contents

4.6.1 Introduction

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`.

```
25 function dudt = patchSmooth2(t,u)
26 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 microscales.
  - `.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 microscales.

Output

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

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

Section 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`.

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

Input

- `u` is a vector of length $\texttt{nx} \cdot \texttt{ny} \cdot \texttt{Nx} \cdot \texttt{Ny} \cdot \texttt{nVars}$ where there are `nVars` field values at each of the points in the $\texttt{nx} \times \texttt{ny} \times \texttt{Nx} \times \texttt{Ny}$ grid on the $\texttt{Nx} \times \texttt{Ny}$ array of patches.
- `patches` a struct set by `configPatches2()` which includes the following information.
  - `.x` is $\texttt{nx} \times \texttt{Nx}$ 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 microscales.
  - `.y` is similarly $\texttt{ny} \times \texttt{Ny}$ 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 microscales.
  - `.ordCC` is order of interpolation, currently only $\{0\}$.
  - `.Cwtsr` and `.Cwtsl`—not yet used

Output

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

Bibliography

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