

# Patch dynamics with buffers for homogenization problems

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*Report TW 411, November 2004*



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## Abstract

An important class of problems exhibits smooth behaviour on macroscopic space and time scales, while only a microscopic evolution law is known. For such time-dependent multi-scale problems, an “equation-free” framework has been proposed, of which patch dynamics is an essential component. Patch dynamics is designed to perform numerical simulations of an unavailable macroscopic equation on macroscopic time and length scales; it uses appropriately initialized simulations of the available microscopic model in a number of small boxes (patches), which cover only a fraction of the space-time domain. To reduce the effect of the artificially introduced box boundaries, we use buffer regions to “shield” the boundary artefacts from the interior of the domain for short time intervals. We analyze the accuracy of this scheme for a diffusion homogenization problem with periodic heterogeneity, and propose a simple heuristic to determine a sufficient buffer size. The algorithm performance is illustrated through a set of numerical examples, which include a non-linear reaction-diffusion equation and the Kuramoto–Sivashinsky equation.

**Keywords :** multiscale computation, equation-free methods, patch dynamics, gap-tooth scheme, homogenization

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# 1 Introduction

For an important class of multi-scale problems, a separation of scales prevails between the (microscopic, detailed) level of description of the available model, and the (macroscopic, continuum) level at which one would like to observe and analyze the system. Consider, for example, a kinetic Monte Carlo model of bacterial growth [31]. A stochastic model describes the probability of an individual bacterium to run or “tumble”, based on the rotation of its flagellae. Technically, it would be possible to simply evolve the detailed model and observe the macroscopic variables of interest (e.g. cell density), but this could be prohibitively expensive. It is known, however, that, under certain conditions, one could write a deterministic equation for the evolution of the macroscopic observable (here *bacteria concentration*, the zeroth moment of the evolving distribution) on macroscopic space and time scales, but it is hard to obtain an accurate closed formula explicitly.

The recently proposed *equation-free framework* [19] can then be used instead of stochastic time integration in the entire space-time domain. This framework is built around the central idea of a *coarse time-stepper*, which is a time- $\delta t$  map from coarse variables to coarse variables. It consists of the following steps: (1) *lifting*, i.e. the creation of *appropriate* initial conditions for the microscopic model; (2) *evolution*, using the microscopic model and (possibly) some constraints; and (3) *restriction*, i.e. the projection of the detailed solution to the macroscopic observation variables. This coarse time-stepper can subsequently be used as “input” for time-stepper based algorithms performing macroscopic numerical analysis tasks. These include, for example, time-stepper based bifurcation codes to perform bifurcation analysis for the *unavailable* macroscopic equation [24, 25, 35, 36]. This approach has already been used in several applications [15, 34], and also allows to perform other system level tasks, such as control and optimization [33].

When dealing with systems that would be described by (in our case, unavailable) *partial* differential equations (PDEs), one can also reduce the *spatial* complexity. For systems with one space dimension, the *gap-tooth scheme* [19] was proposed; it can be generalized in several space dimensions. A number of small intervals, separated by large gaps, are introduced; they qualitatively correspond to mesh points for a traditional, continuum solution of the unavailable equation. In higher space dimensions, these intervals would become *boxes* around the coarse mesh points, a term that we will also use throughout this paper. We construct a coarse time- $\delta t$  map as follows. We first choose a number of macroscopic grid points. Then, we choose a small interval around each grid point; initialize the fine scale, microscopic solver within each interval consistently with the macroscopic initial condition profiles; and provide each box with appropriate boundary conditions. Subsequently, we use the microscopic model in each interval to simulate until time  $\delta t$ , and obtain macroscopic information (e.g. by computing the average density in each box) at time  $\delta t$ . This amounts to a coarse time- $\delta t$  map; the procedure is then repeated. The resulting scheme has already

been used with lattice-Boltzmann simulations of the Fitzhugh–Nagumo dynamics [18, 19] and with particle-based simulations of the viscous Burgers equation [10].

To increase the efficiency of time integration, one can use the gap-tooth scheme in conjunction with any method-of-lines time integration method, such as projective integration [8]. We then perform a number of gap-tooth steps of size  $\delta t$  to obtain an estimate of the time derivative of the unavailable macroscopic equation. This estimate is subsequently used to perform a time step of size  $\Delta t \gg \delta t$ . This combination has been termed *patch dynamics* [19].

In this paper, we will study the patch dynamics scheme for a model diffusion homogenization problem. Here, the microscopic equation is a diffusion equation with a spatially periodic diffusion coefficient with small spatial period  $\epsilon$ , while the macroscopic (effective) equation describes the averaged behaviour. In the limit of  $\epsilon$  going to zero, this effective equation is the classical homogenized equation. Our goal is to approximate the effective equation by using only the microscopic equation in a set of small boxes. In [29], we already studied the gap-tooth scheme for periodic reaction-diffusion homogenization problems. We showed that the gap-tooth scheme approximates a finite difference scheme for the homogenized equation, when the averaged gradient is constrained at the box boundaries. However, generally, a given microscopic code only allows us to run with a set of predefined boundary conditions. It is highly non-trivial to impose macroscopically inspired boundary conditions on such microscopic codes, see e.g. [23] for a control-based strategy. Therefore, we circumvent this problem here by introducing buffer regions at the boundary of each small box, which shield the *short-term* dynamics within the computational domain of interest from boundary effects. One then uses the microscopic code with its *built-in* boundary conditions. In this paper, we study the resulting *gap-tooth scheme with buffers*, which was introduced in [28, 29], when used inside a patch dynamics scheme, and analyze the relation between buffer size, time step and accuracy for a model diffusion homogenization problem. The analysis in this context is important, because we can clearly show the influence of the microscopic scales on the accuracy of the solution for this model problem. However, we emphasize that the real advantage of the method lies in its applicability for non-PDE microscopic simulators, e.g. kinetic Monte Carlo or molecular dynamics.

It is worth mentioning that many numerical schemes have been devised for the homogenization problem. Hou and Wu developed the multi-scale finite element method that uses special basis functions to capture the correct microscopic behaviour [13, 14]. Schwab, Matache and Babuska have devised a generalized FEM method based on a two-scale finite element space [26, 30]. Runborg et al. [27] proposed a time-stepper based method that obtains the effective behaviour through short bursts of detailed simulations appropriately averaged over many shifted initial conditions. The simulations were performed over the whole domain, but the notion of effective behaviour is identical. In their recent work, E and Engquist and collaborators address the same problem of simulating only the macroscopic

behaviour of a multiscale model, see e.g. [1, 7]. In what they call the heterogeneous multiscale method, a macroscale solver is combined with an estimator for quantities that are unknown because the macroscopic equation is not available. This estimator subsequently uses appropriately constrained runs of the microscopic model [7]. It should be clear that patch dynamics does exactly this: by taking a few gap-tooth steps, we estimate the time derivative of the unknown effective equation, and give this as input to an ODE solver, such as projective integration. The difference in their work is that, for conservation laws, the macro-field time derivative is estimated from the *flux* of the conserved quantity; their generalized Godunov scheme is based on this principle.

This paper is organized as follows. In section 2, we describe the model homogenization problem. In section 3, we show how to use the gap-tooth scheme to approximate the time derivative of the unavailable macroscopic equation. We prove a consistency result and propose a simple heuristic to obtain a sufficient buffer size. We also discuss to what extent the results depend on the specific setting of our model problem. In section 4, we describe the full patch dynamics algorithm and give some comments on stability. Section 5 contains some numerical examples which illustrate the accuracy and efficiency of the proposed method, and we conclude in section 6.

## 2 The homogenization problem

As a model problem, we consider the following parabolic partial differential equation,

$$\begin{aligned} \partial_t u_\epsilon(x, t) &= \partial_x (a(x/\epsilon) \partial_x u_\epsilon(x, t)), \quad \text{in } [0, T] \times [0, 1] \\ u_\epsilon(x, 0) &= u^0(x) \in L^2([0, 1]), \quad u_\epsilon(0, t) = u_\epsilon(1, t) = 0, \end{aligned} \quad (1)$$

where  $a(y) = a(x/\epsilon)$  is uniformly elliptic and periodic in  $y$  and  $\epsilon$  is a small parameter. We choose homogeneous Dirichlet boundary conditions for simplicity.

According to classical homogenization theory [5], the solution to (1) can be written as an asymptotic expansion in  $\epsilon$ ,

$$u_\epsilon(x, t) = u_0(x, t) + \sum_{i=1}^{\infty} \epsilon^i (u_i(x, x/\epsilon, t)), \quad (2)$$

where the functions  $u_i(x, y, t) \equiv u_i(x, x/\epsilon, t)$ ,  $i = 1, 2, \dots$  are periodic in  $y$ . Here,  $u_0(x, t)$  is the solution of the *homogenized equation*

$$\begin{aligned} \partial_t u_0(x, t) &= \partial_x (a^* \partial_x u_0(x, t)), \quad \text{in } [0, T] \times [0, 1] \\ u_0(x, 0) &= u^0(x) \in L^2([0, 1]), \quad u_0(0, t) = u_0(1, t) = 0, \end{aligned} \quad (3)$$

the coefficient  $a^*$  is the constant effective coefficient, given by

$$a^* = \int_0^1 a(y) \left( 1 - \frac{d}{dy} \chi(y) \right) dy, \quad (4)$$

and  $\chi(y)$  is the periodic solution of

$$\frac{d}{dy} \left( a(y) \frac{d}{dy} \chi(y) \right) = \frac{d}{dy} a(y), \quad (5)$$

the so-called *cell problem*. The solution of (5) is only defined up to an additive constant, so we impose the extra condition

$$\int_0^1 \chi(y) dy = 0.$$

From this cell problem, we can derive  $u_1(x, y, t) = \partial_x u_0 \chi(y)$ . We note that in one space dimension, an explicit formula is known for  $a^*$ , [5],

$$a^* = \left[ \int_0^1 \frac{1}{a(y)} dy \right]^{-1}. \quad (6)$$

These asymptotic expansions have been rigorously justified in the classical book [5], see also [6]. Under the assumptions made on  $a(x/\epsilon)$ , one obtains strong convergence of  $u_\epsilon(x, t)$  to  $u_0(x, t)$  as  $\epsilon \rightarrow 0$  in  $L^2([0, 1]) \times C([0, T])$ . Indeed, we can write

$$\|u_\epsilon(x, t) - u_0(x, t)\|_{L^2([0, 1])} \leq C_0 \epsilon, \quad (7)$$

uniformly in  $t$ .

It is important to note that the gradient of  $u(x, t)$  is given by

$$\partial_x u_\epsilon(x, t) = \partial_x u_0(x, t) + \partial_y u_1(x, y, t) + O(\epsilon), \quad (8)$$

from which it is clear that the micro-scale fluctuations have a strong effect on the local detailed gradient.

Using the gap-tooth scheme, we will approximate the homogenized solution  $u_0(x, t)$  by a local spatial average, defined as

$$U(x, t) = \mathcal{S}_h(u_\epsilon)(x, t) = \frac{1}{h} \int_{x-h/2}^{x+h/2} u_\epsilon(\xi, t) d\xi.$$

It can easily be seen that that  $U(x, t)$  is a good approximation to  $u_0(x, t)$  in the following sense.

**Lemma 2.1.** *Consider  $u_\epsilon(x, t)$  to be the solution of (1), and  $u_0(x, t)$  to be the solution of the associated homogenized equation (3). Then, assuming*

$$h = O(\epsilon^p), \quad p \in (0, 1), \quad (9)$$

*the difference between the homogenized solution  $u_0(x, t)$  and the averaged solution  $U(x, t)$  is bounded by*

$$\|U(x, t) - u_0(x, t)\|_{L^\infty([0, 1])} \leq C_1 h^2 + C_2 \epsilon^{1-p}. \quad (10)$$

For a proof, we refer to [29, Lemma 3.1]. Note that this error bound can be improved if we have more knowledge about the convergence of  $u_\epsilon$  to  $u_0$  (e.g. in  $L^\infty([0, 1])$ ).

### 3 Estimation of the time derivative

We devise a scheme for the evolution of the averaged behaviour  $U(x, t)$ , while making only use of the given detailed equation (1). Moreover, we assume that a time integration code for (1) has already been written and is available with a number of *standard* boundary conditions, such as no-flux or Dirichlet. We also assume that the order  $d$  of the unavailable macroscopic equation (the highest spatial derivative) is known. A strategy to obtain this information is given in [22]. So, we know that the macroscopic equation is of the form

$$\partial_t U = F(U, \partial_x U, \dots, \partial_x^d U, t), \quad (11)$$

where  $\partial_t$  denotes the time derivative and  $\partial_x^k$  denotes the  $k$ -th spatial derivative.

#### 3.1 The gap-tooth scheme with buffers

Suppose we want to obtain the solution of (11) on the interval  $[0, 1]$ , using an equidistant, macroscopic mesh  $\Pi(\Delta x) := \{0 = x_0 < x_1 = x_0 + \Delta x < \dots < x_N = 1\}$ . For convenience, we define a macroscopic comparison scheme, which is a space-time discretization for (11) in the assumption that this equation is known. We will denote the numerical solution of this scheme by  $U_i^n \approx U(x_i, t_n)$ . Here, we choose as a comparison scheme a forward Euler/spatial finite difference scheme, which is defined by

$$U^{n+\delta} = S(U^n, t_n; \delta t) = U^n + \delta t F(U^n, D^1(U^n), \dots, D^d(U^n), t_n), \quad (12)$$

where  $D^k(U^n)$  denotes a suitable finite difference approximation for the  $k$ -th spatial derivative.

Since equation (11) is not known explicitly, we construct a gap-tooth scheme to approximate the comparison scheme (12). We denote the solution of the gap-tooth scheme by  $\bar{U}_i^n \approx U_i^n$ . The gap-tooth scheme is now constructed as follows. Consider a small interval (box, *tooth*) of length  $h$  around each mesh point, as well as a larger *buffer* interval of size  $H > h$ . (See figure 1.) We will perform a time integration using the microscopic model (1) in each box of size  $H$ , and we provide this simulation with the following initial and boundary conditions.

**Initial condition** We define the initial condition by constructing a local Taylor expansion, based on the (given) box averages  $\bar{U}_i^n$ ,  $i = 0, \dots, N$ , at mesh point  $x_i$  and time  $t_n$ ,

$$\bar{u}^i(x, t_n) = \sum_{k=0}^d D_i^k(\bar{U}^n) \frac{(x - x_i)^k}{k!}, \quad x \in [x_i - \frac{H}{2}, x_i + \frac{H}{2}], \quad (13)$$

where  $d$  is the order of the macroscopic equation. The coefficients  $D_i^k(\bar{U}^n)$ ,  $k > 0$  are the same finite difference approximations for the  $k$ -th spatial derivative that would be used in

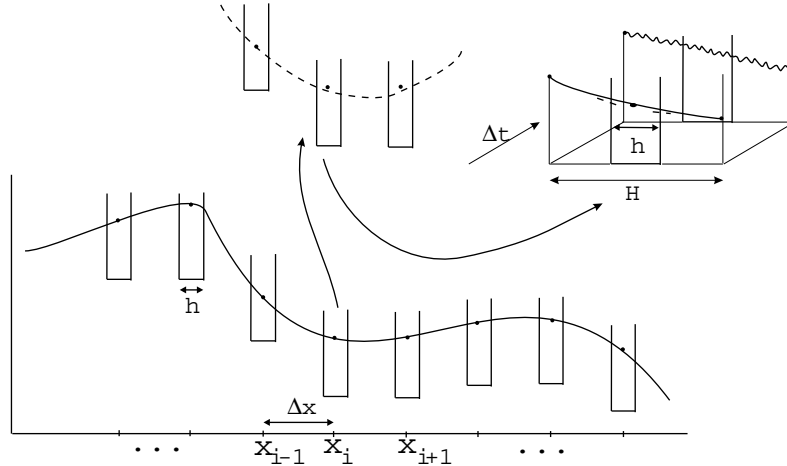


Figure 1: A schematic representation of the gap-tooth scheme with buffer boxes. We choose a number of boxes of size  $h$  around each macroscopic mesh point  $x_i$  and define a local Taylor approximation as initial condition in each box. Simulation is performed inside the larger (buffer) boxes of size  $H$ , where some boundary conditions are imposed.

the comparison scheme (12), whereas  $D_i^0(\bar{U}^n)$  is chosen such that

$$\frac{1}{h} \int_{x_i-h/2}^{x_i+h/2} \bar{u}^i(\xi, t_n) d\xi = \bar{U}_i^n. \quad (14)$$

For example, when  $d = 2$ , and using standard (second-order) central differences, we have

$$D_i^2(\bar{U}^n) = \frac{\bar{U}_{i+1}^n - 2\bar{U}_i^n + \bar{U}_{i-1}^n}{\Delta x^2}, \quad D_i^1(\bar{U}^n) = \frac{\bar{U}_{i+1}^n - \bar{U}_{i-1}^n}{\Delta x}, \quad D_i^0(\bar{U}^n) = \bar{U}_i^n - \frac{h^2}{12} D_i^2(\bar{U}^n). \quad (15)$$

The resulting initial condition was used in [29], where it was derived as an interpolating polynomial for the box averages.

**Boundary conditions** The time integration of the microscopic model in each box should provide information on the evolution of the *global* problem at that location in space. It is therefore crucial that the boundary conditions are chosen such that the solution inside each box evolves *as if it were embedded in the larger domain*. We already mentioned that, in many cases, it is not possible or convenient to impose macroscopically-inspired constraints on the microscopic model (e.g. as boundary conditions). However, we can introduce a larger box of size  $H > h$  around each macroscopic mesh point, but still only use (for macro-purposes) the evolution over the smaller, inner box. The simulation can subsequently be performed using any of the *built-in* boundary conditions of the microscopic code. Lifting and (short-term) evolution (using *arbitrary* available boundary conditions) are performed in the larger box; yet the restriction is done by processing the solution (here taking its average) over the inner, small box only. The goal of the additional computational domains, the *buffers*, is to buffer the solution inside the small box from the artificial disturbance caused by the (repeatedly

updated) boundary conditions. This can be accomplished over *short enough* time intervals, provided the buffers are *large enough*; analyzing the method is tantamount to making these statements quantitative.

The idea of a buffer region was also introduced in the multiscale finite element method of Hou (oversampling) [13] to eliminate boundary layer effects; also Hadjiconstantinou makes use of overlap regions to couple a particle method with a continuum code [12]. If the microscopic code allows a choice of different types of microscopic boundary conditions, selecting the size of the buffer may also depend on this choice.

**The algorithm** The complete gap-tooth algorithm to proceed from  $t_n$  to  $t_n + \delta t$  is given below:

1. **Lifting** At time  $t_n$ , construct the initial condition  $\bar{u}^i(x, t_n)$ ,  $i = 0, \dots, N$  using the box averages  $\bar{U}_i^n$ , as defined in (13).
2. **Simulation** Compute the box solution  $\bar{u}^i(x, t)$ ,  $t > t_n$ , by solving equation (1) in the interval  $[x_i - H/2, x_i + H/2]$  with *some* boundary conditions up to time  $t_{n+\delta} = t_n + \delta t$ . The boundary conditions can be anything that the microscopic code allows.
3. **Restriction** Compute the average  $\bar{U}_i^{n+\delta} = 1/h \int_{x_i-h/2}^{x_i+h/2} \bar{u}^i(\xi, t_{n+\delta}) d\xi$  over the *inner, small box only*.

It is clear that this procedure amounts to a map of the macroscopic variables  $\bar{U}^n$  at time  $t_n$  to the macroscopic variables at time  $t_{n+\delta}$ , i.e. a “coarse to coarse” time  $\delta t$ -map. We write this map as follows,

$$\bar{U}^{n+\delta} = \bar{S}^d(\bar{U}^n, t_n; \delta t, H) = \bar{U}^n + \delta t \bar{F}^d(\bar{U}^n, t_n; \delta t, H), \quad (16)$$

where we introduced the time derivative estimator

$$\bar{F}^d(\bar{U}^n, t_n; \delta t, H) = \frac{\bar{U}^{n+\delta} - \bar{U}^n}{\delta t}. \quad (17)$$

The superscript  $d$  denotes the highest spatial derivative that has been prescribed by the initialization scheme (13). The accuracy of this estimate depends on the buffer size  $H$ , the box size  $h$  and the time step  $\delta t$ .

### 3.2 Consistency

To analyze convergence, we solve the detailed problem approximately in each box. Because  $h \gg \epsilon$ , we can resort to the homogenized solution, and bound the error using equation (7). It is important to note that we use the homogenized equation for analysis purposes only. The algorithm uses box averages of solutions of the detailed problem (1), so it does not

exploit more knowledge of the homogenized equation than the order  $d$ . We choose to study convergence in the case of Dirichlet boundary conditions, but we will show numerically that the results do not depend crucially on the type of boundary conditions.

We first relate the gap-tooth time-stepper as constructed in section 3.1 to a gap-tooth time-stepper in which the microscopic equation has been replaced by the homogenized equation.

**Lemma 3.1.** *Consider the model equation,*

$$\partial_t u_\epsilon(x, t) = \partial_x (a(x/\epsilon) \partial_x u_\epsilon(x, t)), \quad (18)$$

where  $a(y) = a(x/\epsilon)$  is periodic in  $y$  and  $\epsilon \ll 1$ , with initial condition  $u_\epsilon(x, 0) = u^0(x)$  and Dirichlet boundary conditions

$$u_\epsilon(-H/2, t) = u^0(-H/2), \quad u_\epsilon(H/2, t) = u^0(H/2). \quad (19)$$

For  $\epsilon \rightarrow 0$ , this problem converges to the homogenized problem

$$\partial_t u_0(x, t) = \partial_x (a^* \partial_x u_0(x, t)) \quad (20)$$

with initial condition  $u_0(x, 0) = u^0(x)$  and Dirichlet boundary conditions

$$u_\epsilon(-H/2, t) = u^0(-H/2), \quad u_\epsilon(H/2, t) = u^0(H/2). \quad (21)$$

and the solution of (18)-(19) converges pointwise to the solution of (20)-(21), with the following error estimate

$$\|u_\epsilon(x, t) - u_0(x, t)\|_{L^2([-H/2, H/2])} \leq C_3 \epsilon. \quad (22)$$

This is a standard result, whose proof can be found in e.g. [2, 6].

We now define two gap-tooth time-steppers. Let

$$\bar{U}^{n+\delta} = \bar{S}^2(\bar{U}^n, t_n; \delta t, H) = \bar{U}^n + \delta t \bar{F}^2(\bar{U}^n, t_n; \delta t, H) \quad (23)$$

be a gap-tooth time-stepper that uses the detailed, homogenization problem (18)-(19) inside each box, and

$$\hat{U}^{n+\delta} = \hat{S}^2(\hat{U}^n, t_n; \delta t, H) = \hat{U}^n + \delta t \hat{F}^2(\hat{U}^n, t_n; \delta t, H) \quad (24)$$

be a gap-tooth time-stepper where the homogenization problem for each box has been replaced by the homogenized equation (20)-(21). The box initialization is done using a quadratic polynomial as defined in (15).

We can apply [29, Lemma 4.2] to bound the difference between  $\bar{F}^2(\bar{U}, t_n; \delta t, H)$  and  $\hat{F}^2(\hat{U}, t_n; \delta t, H)$ .

**Lemma 3.2.** Consider  $\bar{U}^{n+\delta} = \bar{S}^2(\bar{U}^n, t_n; \delta t, H)$  and  $\hat{U}^{n+\delta} = \hat{S}^2(\hat{U}^n, t_n; \delta t, H)$  as defined in (23) and (24), respectively. Assuming  $\bar{U}^n = \hat{U}^n$ ,  $h = O(\epsilon^p)$ ,  $p \in (0, 1)$ ,  $\epsilon \rightarrow 0$ , we have

$$\left\| \bar{U}_i^{n+\delta} - \hat{U}_i^{n+\delta} \right\| \leq C_4 \epsilon^{1-p/2},$$

and therefore

$$\left\| \bar{F}^2(\bar{U}^n, t_n; \delta t, H) - \hat{F}^2(\hat{U}^n, t_n; \delta t, H) \right\| \leq C_4 \frac{\epsilon^{1-p/2}}{\delta t}.$$

Again, note that the error estimate can be made sharper if additional knowledge of the convergence of  $u_\epsilon$  to  $u_0$  is available.

It can easily be checked that the averaged solution  $U(x, t)$  also satisfies the diffusion equation (20). Therefore, we define the comparison scheme (12) for the model problem as

$$\begin{aligned} U^{n+\delta} &= S(U^n, t_n; \delta t) \\ &= U^n + \delta t F(U^n, D^1(U^n), D^2(U^n), t_n) \\ &= U^n + \delta t [a^* D^2(U^n)]. \end{aligned} \quad (25)$$

The following theorem compares the gap-tooth time derivative estimator  $\hat{F}^2(\hat{U}^n, t_n; \delta t, H)$  with the finite difference time derivative used in (25).

**Theorem 3.3.** Consider the gap-tooth time-stepper for the homogenized equation, as defined by (24), and the corresponding comparison scheme (25). Assuming  $U^n = \hat{U}^n$ , and defining the error

$$E(\delta t, H) = \left\| \hat{F}^2(\hat{U}^n, t_n; \delta t, H) - a^* D^2(U^n) \right\|,$$

we have the following result for  $\delta t/H^2 \rightarrow 0$ ,  $h \ll H$ ,

$$E(\delta t, H) \leq \left( C_1 + C_2 \frac{h^2}{\delta t} \right) \left( 1 - \exp(-a^* \pi^2 \frac{\delta t}{H^2}) \right) \quad (26)$$

*Proof.* First, we solve the equation (20)-(21) analytically inside each box, with initial condition given by (13). Using the technique of separation of variables, we obtain

$$\begin{aligned} \hat{u}^i(x, t) &= \hat{U}_i^n - \frac{h^2}{12} D_i^2(\hat{U}^n) + D_i^2(\hat{U}^n) \frac{H^2}{8} + D_i^1(\hat{U}^n)(x - x_i) \\ &\quad + \sum_{m=1}^{\infty} a_m^i \exp\left(-a^* \frac{m^2 \pi^2}{H^2} (t - t_n)\right) \sin\left(\frac{m\pi}{H} (x - x_i - \frac{H}{2})\right), \end{aligned}$$

where

$$a_m^i = \frac{2}{H} \int_{x_i-H/2}^{x_i+H/2} \frac{1}{2} D_i^2(\hat{U}^n) \left( (x - x_i)^2 - \frac{H^2}{4} \right) \sin\left(\frac{m\pi}{H} (x - x_i - \frac{H}{2})\right) dx.$$

This can be simplified to

$$a_m^i = -\frac{2H^2 D_i^2(\hat{U}^n) ((-1)^m - 1)}{m^3 \pi^3},$$

which yields the following solution,

$$\begin{aligned} \hat{u}^i(x, t) &= \hat{U}_i^n - \frac{h^2}{12} D_i^2(\hat{U}^n) + D_i^2(\hat{U}^n) \frac{H^2}{8} + D_i^1(\hat{U}^n)(x - x_i) \\ &+ \sum_{m=1}^{\infty} \frac{4H^2 D_i^2(\hat{U}^n)}{(2m-1)^3 \pi^3} \exp\left(-a^* \frac{(2m-1)^2 \pi^2}{H^2} (t - t_n)\right) \sin\left(\frac{(2m-1)\pi}{H} (x - x_i - \frac{H}{2})\right). \end{aligned} \quad (27)$$

When taking the average over a box of size  $h$ , we obtain,

$$\begin{aligned} \frac{1}{h} \int_{x_i-h/2}^{x_i+h/2} \hat{u}^i(x, t) dx &= \hat{U}_i^n - \frac{h^2}{12} D_i^2(\hat{U}^n) + D_i^2(\hat{U}^n) \frac{H^2}{8} \\ &+ \sum_{m=1}^{\infty} \frac{4H^2 \alpha_m}{(2m-1)^3 \pi^3} D_i^2(\hat{U}^n) \exp\left(-a^* \frac{(2m-1)^2 \pi^2}{H^2} (t - t_n)\right), \end{aligned} \quad (28)$$

with  $\alpha_m$  determined by

$$\begin{aligned} \alpha_m &= \frac{1}{h} \int_{x_i-h/2}^{x_i+h/2} \sin\left(\frac{(2m-1)\pi}{H} (x - x_i - \frac{H}{2})\right) dx \\ &= \frac{H}{(2m-1)h\pi} \left( \cos\left(\frac{(2m-1)\pi}{2H} (H+h)\right) - \cos\left(\frac{(2m-1)\pi}{2H} (H-h)\right) \right) \\ &= (-1)^m \frac{2H}{(2m-1)h\pi} \sin\left(\frac{(2m-1)\pi}{2H} h\right). \end{aligned}$$

The coefficients  $\alpha_m$  tend to 1 in absolute value as  $h \rightarrow 0$ . To obtain the time derivative estimate  $\hat{F}(\hat{U}^n, t_n; \delta t, H)$ , we proceed as follows:

$$\begin{aligned} \hat{F}_i^2(\hat{U}^n, t_n; \delta t, H) &= \frac{1}{\delta t h} \int_{x_i-h/2}^{x_i+h/2} \hat{u}^i(x, t_n + \delta t) - \hat{u}^i(x, t_n) dx \\ &= \frac{1}{\delta t} \sum_{m=1}^{\infty} \frac{4H^2 \alpha_m}{(2m-1)^3 \pi^3} D_i^2(\hat{U}^n) \left( \exp\left(-a^* \frac{(2m-1)^2 \pi^2}{H^2} \delta t\right) - 1 \right) \\ &= 4D_i^2(\hat{U}^n) \frac{1}{\xi} \left( \sum_{m=1}^{\infty} \frac{\alpha_m (\exp(-a^*(2m-1)^2 \pi^2 \xi) - 1)}{(2m-1)^3 \pi^3} \right) \end{aligned}$$

where we introduced  $\xi = \delta t/H^2$ . It can easily be checked (e.g. using Maple) that

$$\lim_{\xi \rightarrow 0} \hat{F}_i^2(\hat{U}^n, t_n; \delta t, H) = a^* D_i^2(\hat{U}^n),$$

which already shows that the gap-tooth scheme is consistent in this limit. Obtaining an error bound in terms of  $\xi$  is somewhat more involved. We split  $\hat{F}_i^2(\hat{U}^n, t_n; \delta t, H)$  as follows,

$$\hat{F}(\hat{U}^n, t_n; \delta t, H) = \hat{F}_1 + \hat{F}_2,$$

with  $\hat{F}_1$  and  $\hat{F}_2$  defined as

$$\begin{aligned} \hat{F}_1 &= 4D_i^2(\hat{U}^n) \frac{1}{\xi} \left( \sum_{m=1}^{\infty} \frac{(-1)^m (\exp(-a^*(2m-1)^2 \pi^2 \xi) - 1)}{(2m-1)^3 \pi^3} \right) \\ \hat{F}_2 &= 4D_i^2(\hat{U}^n) \frac{1}{\xi} \left( \sum_{m=1}^{\infty} \frac{(\alpha_m - (-1)^m) (\exp(-a^*(2m-1)^2 \pi^2 \xi) - 1)}{(2m-1)^3 \pi^3} \right). \end{aligned}$$

We now show that  $\hat{F}_1$  approaches the correct estimate exponentially. Some algebraic manipulation results in

$$\begin{aligned}\hat{F}_1 - a^* D_i^2(\hat{U}^n) &= 4D_i^2(\hat{U}^n) \frac{1}{\xi} \left( \sum_{m=1}^{\infty} \frac{(-1)^m (\exp(-a^*(2m-1)^2 \pi^2 \xi) - 1)}{(2m-1)^3 \pi^3} \right) - a^* D_i^2(\hat{U}^n) \\ &= 4D_i^2(\hat{U}^n) \sum_{m=1}^{\infty} (-1)^{m+1} \left( \frac{1 - a^*(2m-1)^2 \pi^2 \xi - \exp(-a^*(2m-1)^2 \pi^2 \xi)}{(2m-1)^3 \pi^3 \xi} \right)\end{aligned}$$

Therefore, we have

$$\begin{aligned}\left\| \hat{F}_1 - a^* D_i^2(\hat{U}^n) \right\| &= \\ \left\| 4D_i^2(\hat{U}^n) \sum_{m=1}^{\infty} (-1)^{m+1} a^* \left( \frac{1 - a^*(2m-1)^2 \pi^2 \xi - \exp(-a^*(2m-1)^2 \pi^2 \xi)}{a^*(2m-1)^3 \pi^3 \xi} \right) \right\| & \\ \leq C \left( \frac{1 - a^* \pi^2 \xi - \exp(-a^* \pi^2 \xi)}{a^* \pi^2 \xi} \right) & \\ \leq C (1 - \exp(-a^* \pi^2 \xi)) &\end{aligned} \quad (29)$$

It remains to show the asymptotic behaviour of  $\hat{F}_2$ .

$$\begin{aligned}\left\| \hat{F}_2 \right\| &= \\ \left\| 4D_i^2(\hat{U}^n) \sum_{m=1}^{\infty} (-1)^m \frac{\left( \sin\left(\frac{(2m-1)\pi h}{2H}\right) \frac{2H}{(2m-1)\pi h} - 1 \right)}{(2m-1)^3 \pi^3} \left( \exp(-a^*(2m-1)^2 \pi^2 \xi) - 1 \right) \right\| & \\ \leq C \left( \frac{\sin\left(\frac{\pi h}{2H}\right) \frac{2H}{\pi h} - 1}{\xi \pi^3} \right) (1 - \exp(-a^* \pi^2 \xi)) & \\ \leq C \frac{h^2}{H^2} \frac{1 - \exp(-a^* \pi^2 \xi)}{\xi \pi^3} & \\ \leq C \frac{h^2}{\delta t} (1 - \exp(-a^* \pi^2 \xi)) &\end{aligned} \quad (30)$$

The combination of (29) and (30) proves the theorem.  $\square$

The error bound (26) clearly shows an exponential decay of the error as a function of  $\delta t/H^2$  when the microscopic problem is replaced by the effective equation. The restriction (here performed by taking the box average) also affects the accuracy of the estimate. Ideally, one would just use the effective function value at  $x = x_i$  inside each box (this corresponds to  $h = 0$ ), but when microscopic scales are present, this value is generally impossible to obtain.

We illustrate this result numerically.

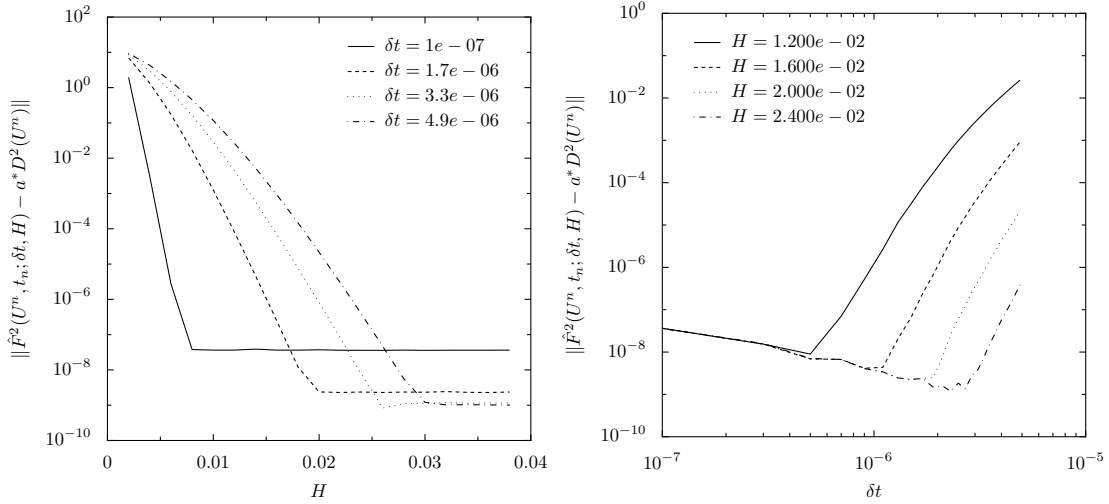


Figure 2: Error of the gap-tooth estimator  $\hat{F}^2(U^n, t_n; \delta t, H)$  (which uses the homogenized problem (20)-(21) inside each box) with respect to the finite difference time derivative  $a^* D^2(U^n)$  on the same mesh. Left: Error with respect to  $H$  for fixed  $\delta t$ . Right: Error with respect to  $\delta t$  for fixed  $H$ .

**Example 3.4.** Consider the model problem (20) with  $a^* = 0.45825686$  as a microscopic problem on the domain  $[0, 1]$  with homogeneous Dirichlet boundary conditions and initial condition  $u(x, 0) = 1 - 4(x - 1/2)^2$ . To solve this microscopic problem, we use a second order finite difference discretization with mesh width  $\delta x = 2 \cdot 10^{-7}$  and `lsode` as time-stepper. The concrete gap-tooth scheme for this example is defined by the initialization (15). We compare a gap-tooth step with  $h = 2 \cdot 10^{-3}$  and  $\Delta x = 1 \cdot 10^{-1}$  with the reference estimator  $a^* D^2(\hat{U}^n)$ . Figure 2 shows the error with respect to the finite difference time derivative as a function of  $H$  (left) and  $\delta t$  (right). It is clear the convergence is in agreement with theorem 3.3. The stagnation for large buffer sizes is due to the finite accuracy of the microscopic solver.

We are now ready to state the general consistency result.

**Theorem 3.5.** Let  $\bar{U}^{n+\delta} = \bar{S}^2(\bar{U}^n, t_n; \delta t, H)$  be a gap-tooth time-stepper for the homogenization problem (18)-(19), as defined in (23), and  $U^{n+\delta} = S(U^n, t_n; \delta t)$  a comparison finite difference scheme as defined in (25). Then, assuming  $U^n = \bar{U}^n$ , we have,

$$\|\bar{F}^2(\bar{U}^n, t_n; \delta t, H) - a^* D^2(U^n)\| \leq C_4 \underbrace{\frac{\epsilon^{1-p/2}}{\delta t}}_{\text{microscales}} + C_5 \underbrace{\left(1 + \frac{h^2}{\delta t}\right)}_{\text{averaging}} \underbrace{\left(1 - \exp\left(-a^* \pi^2 \frac{\delta t}{H^2}\right)\right)}_{\text{boundary conditions}} \quad (31)$$

*Proof.* This simply follows by combining theorem 3.3 with lemma 3.1.  $\square$

Formula (31) shows the main consistency properties of the gap-tooth estimator. The

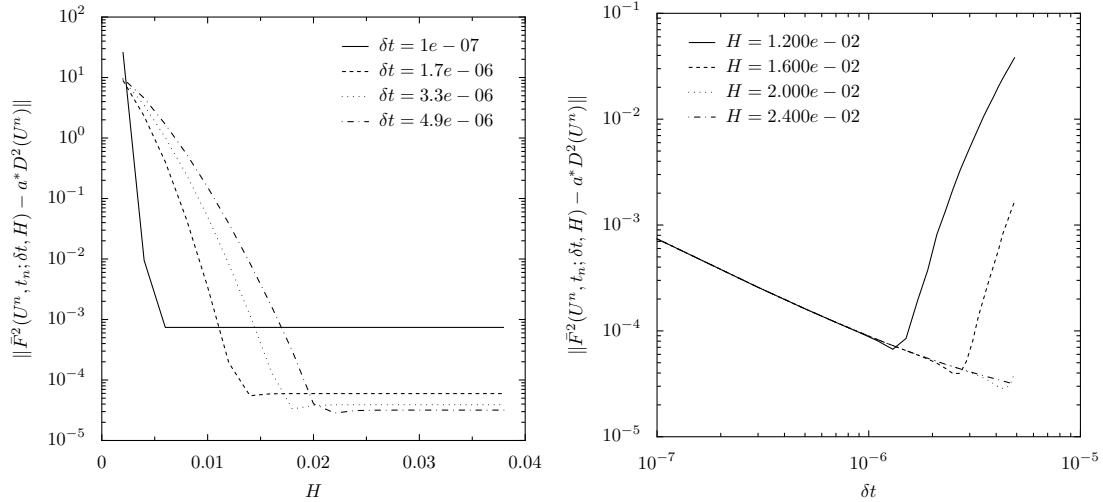


Figure 3: Error of the gap-tooth estimator  $\bar{F}(U^n, t_n; \delta t, H)$  (which uses the detailed, homogenization problem (18)–(19) inside each box) with respect to the finite difference time derivative  $a^* D^2(U^n)$  on the same mesh. Left: Error with respect to  $H$  for fixed  $\delta t$ . Right: Error with respect to  $\delta t$  with fixed  $H$ .

error decays exponentially as a function of buffer size, but the optimal accuracy of the estimator is limited by the presence of the microscopic scales. Therefore, we need to make a trade-off to determine an optimal choice for  $H$  and  $\delta t$ . The smaller  $\delta t$ , the smaller  $H$  can be to reach optimal accuracy (and thus the smaller the computational cost), but smaller  $\delta t$  implies a larger optimal error. This is illustrated in the following numerical example.

**Example 3.6.** Consider the model problem (18) with

$$a(x/\epsilon) = 1.1 + \sin(2\pi x/\epsilon), \quad \epsilon = 1 \cdot 10^{-5} \quad (32)$$

as a microscopic problem on the domain  $[0, 1]$  with homogeneous Dirichlet boundary conditions and initial condition  $u(x, 0) = 1 - 4(x - 1/2)^2$ . This diffusion coefficient has also been used as a model example in [1, 29]. To solve this microscopic problem, we use a second order finite difference discretization with mesh width  $\delta x = 1 \cdot 10^{-7}$  and `lsode` as time-stepper. The concrete gap-tooth scheme for this example is defined by the initialization (15). We compare a gap-tooth step with  $h = 2 \cdot 10^{-3}$  and  $\Delta x = 1 \cdot 10^{-1}$  with the reference estimator  $a^* D^2(\hat{U}^n)$ , in which the effective diffusion coefficient is known to be  $a^* = 0.45825686$ . Figure 3 shows the error with respect to the finite difference time derivative as a function of  $H$  (left) and  $\delta t$  (right). It is clear that the convergence is in agreement with theorem 3.5. We see that smaller values of  $\delta t$  result in larger values for the optimal error, but the convergence towards this optimal error is faster.

### 3.3 Choosing the method parameters

When performing time integration using patch dynamics, one must determine a macroscopic mesh width  $\Delta x$ , an inner box size  $h$ , a buffer box size  $H$  and a time step  $\delta t$ . These method parameters need to be chosen adequately to ensure an accurate result. Since the gap-tooth estimator approximates the time derivative that would be obtained through a method-of-lines discretization of the macroscopic equation, the macroscopic mesh width  $\Delta x$  can be determined by macroscopic properties of the solution only, enabling reuse of existing remeshing techniques for PDEs. The box width  $h$  has to be sufficiently large to capture all small scale effects, but small enough to ensure a good spatial resolution. Here, we just choose  $h \gg \epsilon$ . In our simplified setting, where the microscopic model is also a partial differential equation, we are free to choose  $\delta t$ , which allows us to illustrate the convergence properties of the method. However, in practical problems, the choice of  $\delta t$  will be problem-dependent, since it will need to be chosen large enough to deduce reliable information on the macroscopic time derivative.

Therefore, we focus on determining the buffer width  $H$ , assuming that all other parameters have already been fixed. From theorem 3.5, it follows that the desired value of  $H$  depends on the effective diffusion coefficient  $a^*$ , which is unknown. We thus need to resort to a heuristic. Consider the model problem (18)-(19) inside one box, centered around  $x_0 = 5 \cdot 10^{-1}$ , with  $H = 8 \cdot 10^{-3}$ , with initial condition  $u^0(x) = 1 - 4(x - 1/2)^2$ . The diffusion coefficient is given by (32), see example 3.6. Denote the solution of this problem by  $\bar{u}(x, t)$ , and define

$$\begin{aligned} \bar{F}(x, t) &= \mathcal{S}_h(\bar{u}(x, t) - \bar{u}(x, 0)) \\ &= \frac{1}{t} \int_{\xi - x_0 - h/2}^{\xi - x_0 + h/2} \frac{\bar{u}(\xi, t) - \bar{u}(\xi, 0)}{h} d\xi, \end{aligned} \quad (33)$$

with  $h = 2 \cdot 10^{-3}$  and  $x \in [(-H + h)/2, (H - h)/2]$ . Figure 4 (left) shows  $\bar{F}(x, t)$  for a number of values of  $t$ . We clearly see how the error in the estimator propagates inwards from the boundaries. The same function is plotted on the right, only now the microscopic model is the reaction-diffusion equation

$$\begin{aligned} \partial_t u_\epsilon(x, t) &= \partial_x (a(x/\epsilon) \partial_x u_\epsilon(x, t)) + u_\epsilon(x, t) \left( 1 - \frac{u_\epsilon(x, t)}{1.2 + \sin(2\pi x)} \right) \\ u_\epsilon(-H/2, t) &= u^0(-H/2), \quad u_\epsilon(H/2, t) = u^0(H/2), \end{aligned} \quad (34)$$

again with  $a(x/\epsilon)$  defined as in (32). In the presence of reaction terms,  $\bar{F}(x, t)$  is no longer constant in the internal region. Based on these observations, we propose the following test for the quality of the buffer size,

$$\|\bar{F}(0, \delta t) - \bar{F}(0, (1 - \alpha)\delta t)\| < \text{Tr}, \quad 0 < \alpha \ll 1. \quad (35)$$

Figure 5 shows this heuristic, together with the error, as a function of  $H$  for  $\delta t = 5 \cdot 10^{-6}$  and  $\alpha = 0.04$ . It is clear that the computed quantity in (35) is proportional to the error for

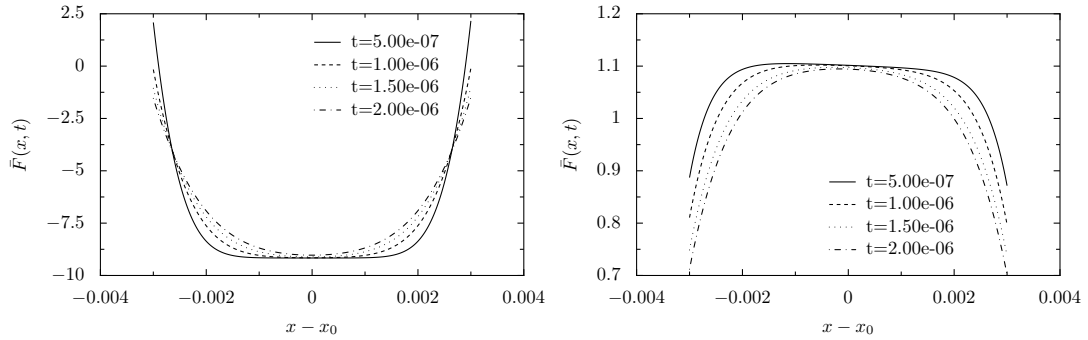


Figure 4: The function  $\bar{F}(x, t)$  as defined in equation (33) for a number of values of time, using a buffer size  $H = 8 \cdot 10^{-3}$  and  $h = 2 \cdot 10^{-3}$ . Left: the model diffusion problem (18-19). Right: the reaction-diffusion equation 34. The estimate clearly gets affected by the boundary conditions as time advances.

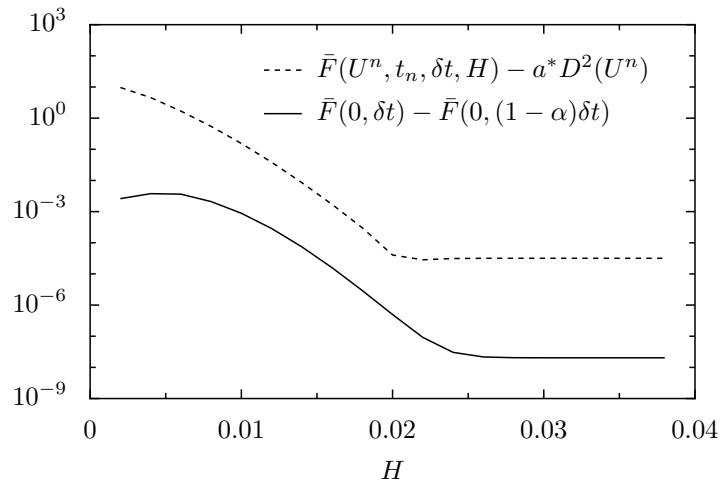


Figure 5: Error of the gap-tooth estimator (dashed) and heuristic error estimate (solid) as a function of buffer size for the model equation (18) with diffusion coefficient (32) for  $\delta t = 5 \cdot 10^{-6}$  and  $\alpha = 0.04$ .

sufficiently large  $H$ . However, this heuristic is far from perfect, since the simulations inside each box can converge to a steady state due to the Dirichlet boundary conditions. If this steady state is reached in a time interval smaller than  $\delta t$ , equation (35) will underestimate the error, resulting in an insufficient buffer size  $H$  getting accepted. However, as soon as the problem-dependent parameters  $\alpha$  and  $\text{Tr}$  have been determined, this heuristic can be used during the simulation to check whether the currently used buffer size is still sufficient.

### 3.4 Discussion

**Other boundary conditions** In section 3.2, we studied the convergence of the gap-tooth estimator both analytically and numerically in the case of Dirichlet boundary conditions. We will now show numerically that the results obtained in that section do not depend crucially on the type of boundary conditions. Consider again the diffusion problem (18), with the diffusion coefficient defined as in (32), see also example 3.6. We construct the gap-tooth time derivative estimator  $\bar{F}(U^n, t_n; \delta t, H)$  as outlined in section 3.1, but now we use no-flux instead of Dirichlet boundary conditions. In each box, we then solve the following problem,

$$\begin{aligned} \partial_t u_\epsilon(x, t) &= \partial_x (a(x/\epsilon) \partial_x u_\epsilon(x, t)), \\ \partial_x u_\epsilon(-H/2, t) &= 0, \quad \partial_x u_\epsilon(H/2, t) = 0 \end{aligned} \tag{36}$$

The concrete gap-tooth scheme that is used, as well as the corresponding finite difference comparison scheme, are defined by the initialization (15). Figure 6 shows the error with respect to the finite difference time derivative  $a^* D^2(U^n)$ . We see qualitatively the same behaviour as for Dirichlet boundary conditions.

In general, the choice of boundary conditions might influence the required buffer size. In the ideal case, where the boundary conditions are chosen to correctly mimic the behaviour in the full domain, we can choose  $H = h$ . Then there is no buffer and the computational complexity is, in some sense, optimal. For reaction-diffusion homogenization problems, this can be achieved by constraining the averaged gradient around each box edge [29]. In situations where the correct boundary conditions are not known, or prove impossible to implement, one is forced to resort to the use of buffers.

**Microscopic simulators** It is possible that the microscopic model is not a partial differential equation, but some microscopic simulator, e.g. kinetic Monte Carlo or molecular dynamics code. In fact, this is the case where we expect our method to be most useful. In this case, the *lifting* step, i.e. the construction of box initial conditions, becomes more involved. In general, the microscopic model will have many more degrees of freedom, the *higher order moments* of the evolving distribution. These will quickly become slaved to the governing moments (the ones where the lifting is conditioned upon), see e.g. [19, 24]. The

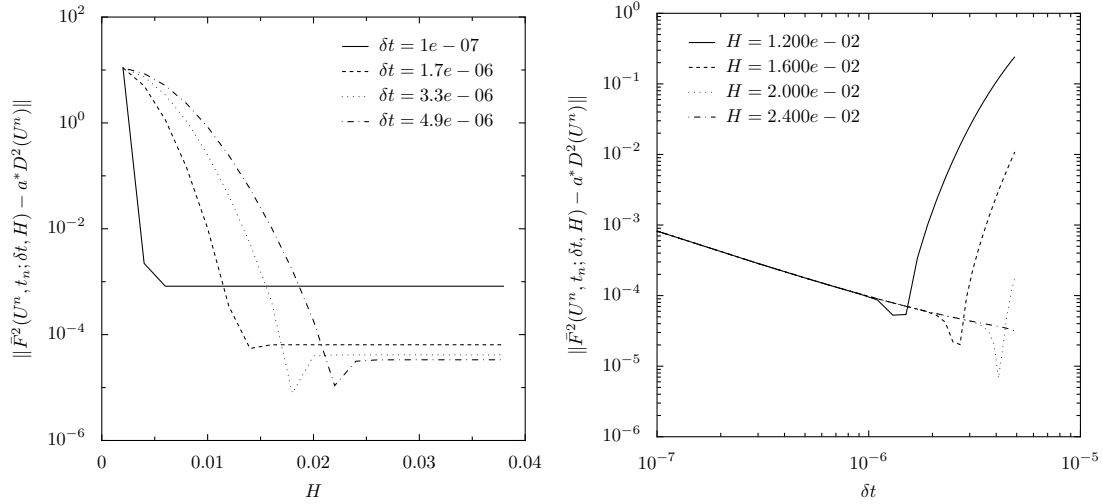


Figure 6: Error of the gap-tooth estimator  $\bar{F}(U^n, t_n; \delta t, H)$  (using the microscopic problem (36) with diffusion coefficient (32) in each box) with respect to the finite difference time derivative  $a^* D^2(U^n)$  on the same mesh.

crucial assumption in theorem 3.5 is that the solution in each box evolves according to the macroscopic equation. For a microscopic simulation, this will usually mean that we need to construct an initial condition in which, for example, a number of higher order moments are already slaved to the governing moments (so-called *mature* initial conditions). To this end, it is possible to perform a constrained simulation before initialization to create such *mature* initial conditions [9, 15]. If this is not done, the resulting evolution may be far from what is expected, see [21] for an illustration in the case of a lattice-Boltzmann model.

## 4 Patch dynamics

Once a good gap-tooth time derivative estimator has been constructed, it can be used as a method-of-lines spatial discretization in conjunction with any time integration scheme. Consider for concreteness the forward Euler scheme for (11), given by

$$U^{n+1} = U^n + \Delta t F(U^n, D^1(U^n), \dots, D^d(U^n), t_n), \quad (37)$$

which we will abbreviate as

$$U^{n+1} = U^n + \Delta t F(U^n, t_n) \quad (38)$$

and the corresponding patch dynamics scheme

$$\bar{U}^{n+1} = \bar{U}^n + \Delta t \bar{F}^d(\bar{U}^n, t_n; \delta t, H), \quad (39)$$

where  $\bar{F}^d(\bar{U}^n, t_n; \delta t, H)$  is defined as in (17). Theorem 3.5 establishes the consistency of the gap-tooth estimator. In order to obtain convergence, we also need to prove stability. For this purpose, we define the class  $K$  of discrete functions with bounded divided differences up to order  $d$  on the numerical grid  $(x_i, t_n)$ ,  $i = 0, \dots, N$ ;  $t_n = n\Delta t$ ,  $n = 0, \dots, T/\Delta t$ , as

$$K = \{\{U_i^n\} \mid \|D_{\Delta x}^\alpha U_i^n\| \leq C_\alpha \text{ for } \alpha \leq d, n\Delta t \leq T\},$$

where  $d$  is the highest spatial derivative present in equation (11),  $D_{\Delta x}^\alpha$  is the finite difference operator of order  $\alpha$  on a mesh of width  $\Delta x$ , and  $C_\alpha$  is independent of  $\Delta t$  and  $\Delta x$ . We can then make use of [7, Theorem 5.5] to state the following result. (See also [29, Theorem 4.5] in the case of constrained gradient boundary conditions.)

**Theorem 4.1.** *Consider the patch dynamics scheme (39) and the corresponding finite difference comparison scheme (37). Assume that  $\{\bar{U}^n\}$ ,  $\{U^n\}$ ,  $\{\hat{U}^n\} \in K$ ,  $U^0 = \hat{U}^0 = \bar{U}^0$  and the comparison scheme (37) is stable, then we have*

$$\|\bar{U}^n - u_0(x_i, t_n)\| \leq C_1(\Delta x^k + \Delta t) + C_2 \max_{0 \leq k \leq T/\Delta t} \|\bar{F}^d(\bar{U}^n, t_n; \delta t, H) - F(U^n, t_n)\|.$$

in the limit where

$$\|\bar{F}^d(\bar{U}^n, t_n; \delta t, H) - F(U^n, t_n)\| \rightarrow 0.$$

Thus the patch dynamics scheme is stable if the finite difference comparison scheme is stable. We note that, although this result is very general, its applicability is limited due to the assumption that  $\bar{U}^n \in K$ , which has to be checked separately. Therefore, this result does not prevent the patch dynamics scheme to become unstable, due to e.g. an insufficient buffer size  $H$ . However, we can study the stability of the patch dynamics scheme numerically by computing the eigenvalues of the time derivative estimator as a function of  $H$ .

Consider the homogenization diffusion equation (18) with the diffusion coefficient  $a(x/\epsilon)$  given by (32). The homogenized equation is given by (20) with  $a^* = 0.45825686$ . In this case, the time derivative operator  $F(U^n, t_n)$  in the comparison scheme (37) has eigenvalues

$$\lambda_k = -\frac{4a^*}{\Delta x^2} \sin^2(\pi k \Delta x), \quad (40)$$

which, using the forward Euler scheme as time-stepper, results in the stability condition

$$\max_k |1 + \lambda_k \Delta t| \leq 1 \quad \text{or} \quad \frac{\Delta t}{\Delta x^2} \leq \frac{1}{2} a^*$$

It can easily be checked that the operator  $\bar{F}(U^n, t_n; \delta t, H)$  is linear, so we can interpret the evaluation of  $\bar{F}(U^n, t_n; \delta t, H)$  as a matrix-vector product. We can therefore use any matrix-free linear algebra technique to compute the eigenvalues of  $\bar{F}(U^n, t_n; \delta t, H)$ , e.g. Arnoldi. We choose to compute  $\bar{F}(U^n, t_n; \delta t, H)$  and  $F(U^n, t_n)$  on the domain  $[0, 1]$  with Dirichlet boundary conditions, on a mesh of width  $\Delta x = 0.05$  and with an inner box width of  $h = 2 \cdot 10^{-3}$ . We choose  $\delta t = 5 \cdot 10^{-6}$  and compute the eigenvalues of  $\bar{F}(U^n, t_n; \delta t, H)$  as

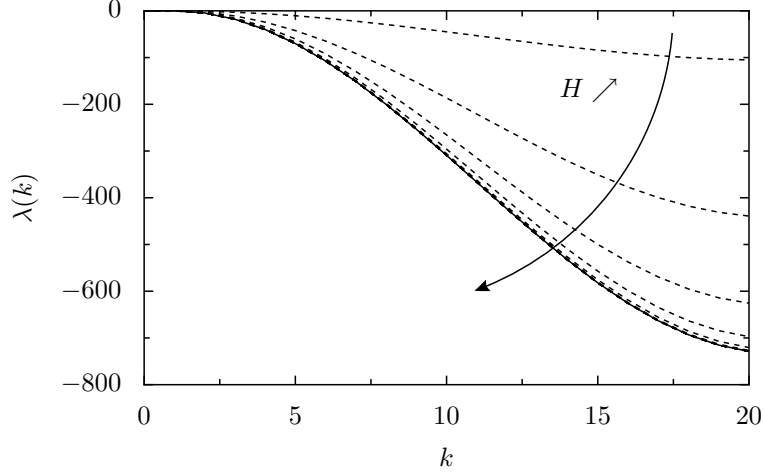


Figure 7: Spectrum of the estimator  $\bar{F}(U^n, t_n; \delta t, H)$  (dashed) for the model equation (18) with diffusion coefficient (32) for  $H = 2 \cdot 10^{-3}, 4 \cdot 10^{-3}, \dots, 2 \cdot 10^{-2}$  and  $\delta t = 5 \cdot 10^{-6}$ , and the eigenvalues (40) of  $F(U^n, t_n)$  (solid).

a function of  $H$ . The results are shown in figure 7. Two conclusions are apparent: since the most negative eigenvalue for  $\bar{F}(U^n, t_n; \delta t, H)$  is always smaller in absolute value than the corresponding eigenvalue of  $F(U^n, t_n)$  the patch dynamics scheme is always stable if the comparison scheme is stable. Moreover, we see that, with increasing buffer size  $H$ , the eigenvalues of  $\bar{F}(U^n, t_n; \delta t, H)$  approximate those of  $F(U^n, t_n)$ , which is an indication of consistency.

## 5 Numerical results

We will consider two example systems to illustrate the method. The first example is a system of two coupled reaction-diffusion equations, which models CO oxidation on a heterogeneous catalytic surface. Due to the reaction term, the proof of theorem 3.5 is strictly speaking not valid, but nevertheless the conclusions are the same. The second example is the Kuramoto–Sivashinsky equation. This fourth-order non-linear parabolic equation is widely used e.g. in combustion modeling. The patch dynamics scheme with buffers also works in this case, showing the more general applicability of the method. All computations were performed in Python, making use of the SciPy package [16] for scientific computing.

## 5.1 Example 1: A nonlinear travelling wave in a heterogeneous excitable medium

Consider the following system of two coupled reaction-diffusion equations,

$$\begin{aligned}\partial_t u(x, t) &= \partial_x^2 u(x, t) + \frac{1}{\delta} u(x, t)(1 - u(x, t)) \left( u(x, t) - \frac{w(x, t) + b(x)}{a(x)} \right), \\ \partial_t w(x, t) &= g(u(x, t)) - w(x, t),\end{aligned}\tag{41}$$

with

$$g(u) = \begin{cases} 0, & u < 1/3, \\ 1 - 6.75 u(1 - u)^2, & 1/3 \leq u < 1, \\ 1, & u \geq 1. \end{cases}\tag{42}$$

This equation models the spatiotemporal dynamics of CO oxidation on microstructured catalysts, which consist of, say, alternating stripes of two different catalysts, such as platinum, Pt, and palladium, Pd, or platinum and rhodium, Rh [11, 4, 32]. The goal is to improve the average reactivity or selectivity by combining the catalytic activities of the different metals, which are coupled through surface diffusion. In the above model,  $u$  corresponds to the surface concentration of CO,  $w$  is a so-called surface reconstruction variable and  $g(u)$  is an experimentally fitted sigmoidal function. Details can be found in [17, 3].

In this model  $a$  and  $b$  and the time-scale ratio parameter  $\delta$  are physical parameters that incorporate the experimental conditions: partial pressures of O<sub>2</sub> and CO in the gas phase, temperature, as well as kinetic constants for the surface. Here, we will study a domain of length  $L = 21$  with a periodically varying medium: a striped surface that can be thought of as consisting of equal amounts of Pt and Rh, with stripe width  $\epsilon/2$ . The medium is then defined by

$$a(x) = 0.84, \quad b(x) = -0.025 + 0.725 \sin(2\pi x/\epsilon), \quad \delta = 0.025.\tag{43}$$

This particular choice of parameters is taken from [27], where an effective bifurcation analysis for this model was presented. For these parameter values, the effective equation (given by (41)-(42) with

$$a(x) = 0.84, \quad b(x) = -0.025, \quad \delta = 0.025,\tag{44}$$

supports travelling waves. It was shown in [27] that this conclusion remains true for the given heterogeneity. This was done by computing the effective behaviour as the average of a large number of spatially shifted realization of the wave. Here, using the gap-tooth scheme, the solution is spatially averaged inside each box, but the notion of effective behaviour is identical. We choose the small scale parameter  $\epsilon = 1 \cdot 10^{-4}$ .

The macroscopic comparison scheme for the effective equation (41-42)-(44) is defined as a standard second order central difference discretization in space on a macroscopic mesh of

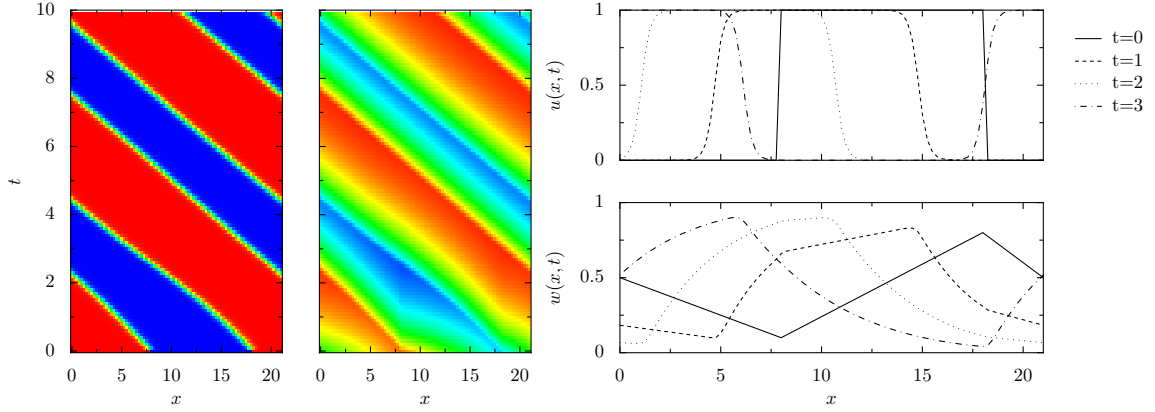


Figure 8: Left: solution of equation (41-43) using the patch dynamics scheme as a function of space and time. Colors indicate values (blue = 1, red = 0). Right: snapshots of the solution at certain moments in time, clearly showing the approach to a travelling wave solution.

width  $\Delta x = 0.25$ , combined with a forward Euler time-stepper. The time-step is chosen as  $\Delta t = 1 \cdot 10^{-2}$ , which ensures stability. The patch dynamics scheme for the detailed equation (41-43) is then obtained by using a gap-tooth estimator for the time derivative using the initialization (15) with the same forward Euler time-stepper.

**Accuracy** We perform a numerical simulation for this model on the domain  $[0, L]$  using the patch dynamics scheme. The gap-tooth parameters are given by  $h = 5 \cdot 10^{-4}$ ,  $H = 1.5 \cdot 10^{-2}$  and  $\delta t = 5 \cdot 10^{-7}$ . Inside each box, we used a finite difference approximation in space, with mesh width  $\delta x = 1 \cdot 10^{-6}$  and `lsode` as time-stepper. The initial condition is given by

$$u(x, 0) = \begin{cases} 1, & x \in [8, 18] \\ 0, & \text{else} \end{cases} \quad w(x, 0) = \begin{cases} 0.5 - 0.05x, & x \leq 8, \\ 0.07x - 0.46, & 8 < x \leq 18, \\ -0.1x + 2.6, & x > 18. \end{cases}$$

The results are shown in figure 8. We clearly see both the initial transient and the final travelling wave solution. For comparison purposes, the same computation was performed using the finite difference comparison scheme for the effective equation. We also computed an “exact” solution for the effective equation using a much finer grid ( $\Delta x = 5 \cdot 10^{-3}$  and  $\Delta t = 1 \cdot 10^{-5}$ ). Figure 9 shows the errors of the patch dynamics simulation with respect to the finite difference simulation of the effective equation and the “exact” solution, respectively. We clearly see that the patch dynamics scheme is a very good approximation of the finite difference scheme, and the error with respect to the exact solution is dominated by the error of the finite difference scheme.

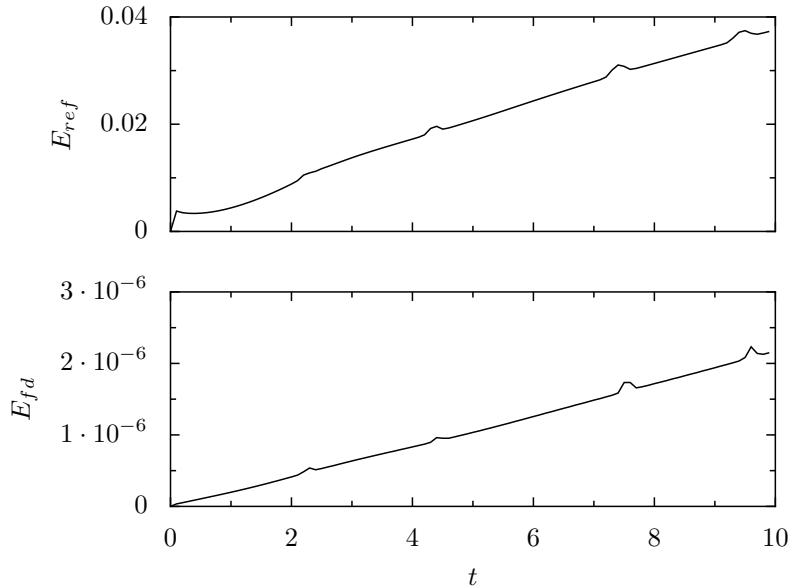


Figure 9: Error of a patch dynamics simulation for equation (41-43) with respect to the “exact” solution of the effective equation (top) and a finite difference comparison scheme (bottom). The error is dominated by the error of the finite difference scheme.

**Efficiency** Time integration using the patch dynamics scheme is more efficient than a complete simulation using the microscopic model, since the microscopic model is used only in small portions of the space-time domain (the patches). An obvious (but not always correct) way to study the efficiency is to compare the size of the total space-time domain with the size of the patches. In this example, the simulations are only performed in 6% of the spatial domain. Of course, when it is possible to apply physically correct boundary conditions around the inner box, the buffer boxes are not necessary, and the boxes would only cover 0.2 % of the space domain. For reaction-diffusion homogenization problems, we showed that buffer boxes are not required when we constrain the average gradient at the box boundary [29]. The gain in the spatial dimension is determined by the separation in spatial scales. It can be large when the macroscopic solution is smooth (few macroscopic mesh points are needed) and propagation of boundary artefacts is slow (small buffer box is sufficient). Note that in higher spatial dimensions, this gain can be even more spectacular.

The gain in the temporal dimension can be determined similarly. In the example of section 5.1, the gap-tooth step was chosen as  $\delta t = 5 \cdot 10^{-7}$ , whereas for macroscopic time integration, the forward Euler scheme was used with  $\Delta t = 1 \cdot 10^{-2}$ . Therefore, in the temporal dimension, we gain a factor of  $2 \cdot 10^5$ . In more realistic applications, when the microscopic model is not a partial differential equation, we expect this gain to be smaller, since additional computational effort will be required to remove the errors that were introduced during the lifting step, e.g. in the form of constrained simulation [9].

## 5.2 Example 2: Kuramoto–Sivashinsky equation

Consider the Kuramoto–Sivashinsky equation

$$\partial_t u(x, t) = -\nu \partial_x^4 u(x, t) - \partial_x^2 u(x, t) - u(x, t) \partial_x u(x, t), \quad x \in [0, 2\pi], \quad (45)$$

with periodic boundary conditions. This equation is frequently used in the modelling of combustion and thin film flow. For the parameter value  $\nu = 4/15$ , it has been shown that the equation supports travelling wave solutions, see e.g. [20]. For the purpose of this example, both the microscopic and the macroscopic model are given by (45).

To obtain the macroscopic comparison scheme, we discretize the second and fourth order spatial derivatives using second order central differences, on a macroscopic mesh of width  $\Delta x = 0.05\pi$ , combined with a forward Euler time integrator with time-step  $\Delta t = 1 \cdot 10^{-5}$ . This small macroscopic time-step arises due to the stiffness of the effective equation. We can accelerate time-stepping by wrapping a so-called *projective integration method* around the forward Euler scheme [8]. This scheme works as follows. First, we perform a number of forward Euler steps,

$$U^{k+1, N} = U^{k, N} + \Delta t F(U^{k, N}, t_n),$$

where, for consistency,  $U^{0, N} = U^N$ , followed by a large extrapolation step

$$U^{N+1} = (M + 1) U^{k+1, N} - M U^{k, N}, \quad M > k.$$

Here,  $U^{k, N} \approx U(N (M + k + 1) \Delta t + k \Delta t)$ . The parameters  $k$  and  $M$  determine the stability region of the resulting time-stepper. An analysis of these methods is given in [8]. It can be checked that, for this equation, choosing  $k = 2$  and  $M = 7$  results in a stable time-stepping scheme.

The patch dynamics scheme is constructed by replacing the time derivative  $F(U^{k, N}, t_n)$  by a gap-tooth estimator  $\bar{F}^4(\bar{U}^{k, N}, t_n; \delta t, H)$ , obtained by the initialization (13), where we choose the order of the Taylor expansion to be  $d = 4$ . The coefficients  $D_k^i$ ,  $k > 0$  are determined by the macroscopic comparison scheme. Inside each box, equation (45) is solved, on a mesh of width  $\delta x = 1 \cdot 10^{-5}$ , subject to Dirichlet and no-flux boundary conditions, using `lsode` as time-stepper. We fixed the box width  $h = 1 \cdot 10^{-3}$ .

**Consistency and efficiency** Because of the fourth order term, theorem 3.5 is not proven. Therefore, we numerically check the consistency of the estimator, by computing the gap-tooth estimator  $\bar{F}^4(\bar{U}^{k, N}, t_n; \delta t, H)$  as a function of  $H$  for a range of values for  $\delta t$ , and comparing the resulting estimate with the time derivative of the comparison scheme. As an initial condition, we choose  $u^0(x) = \sin(2\pi x)$ . The results are shown in figure 10 (left). We see qualitatively the same behaviour as in section 3.2 for diffusion problems.

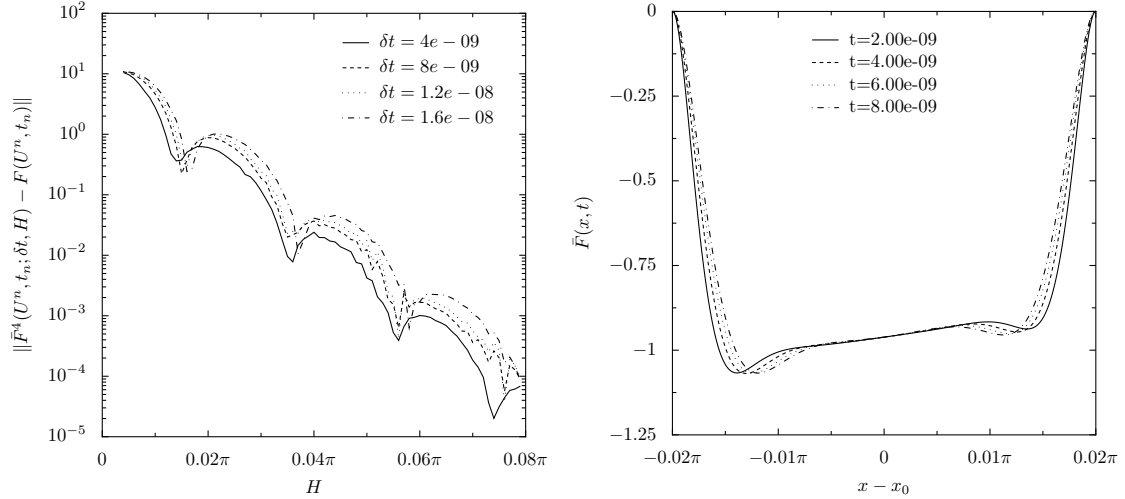


Figure 10: Left: Error of the gap-tooth estimator  $\bar{F}(\bar{U}^{0,0}, t_n; \delta t, H)$  with respect to the finite difference time derivative  $F(U^{0,0}, t_n)$ . Right: The function (33) as a function of  $x$  for a number of values of time. We clearly see how the estimate gets affected by the boundary conditions.

There are two main differences. First, in this case the convergence is no longer monotonic, which explains the sharp peaks in the error curves. Also, because boundary artefacts travel inwards much faster, the gain will be much smaller. Indeed, the figure suggests that a good compromise between accuracy and efficiency would be to choose  $\delta t = 4 \cdot 10^{-9}$  and  $H = 3\pi \cdot 10^{-2}$ . The reason for this behaviour is that the macroscopic equation contains reasonably fast time scales. Note that this is also the reason why the finite difference comparison scheme is forced to take small time-steps.

For this choice of the parameters, the computations have to be performed in 60% of the spatial domain. However, for a forward Euler step, we only need to simulate in  $1/25000$  of the time-domain. Using the projective integration scheme therefore gives us a total gain factor of about 80000 in time. Again, we note that in real applications, this spectacular gain will partly be compensated by the additional computational effort that is required to create appropriate initial conditions.

We can draw two main conclusions. The scheme allows to simulate higher order macroscopic equations, and the gain in the space domain is heavily dependent on the separation of scales in the macroscopic equation.

**Accuracy** We perform a numerical simulation for this model on the domain  $[0, 2\pi]$  using the patch dynamics scheme. The gap-tooth parameters are given by  $h = 1 \cdot 10^{-3}$ ,  $H = 3\pi \cdot 10^{-2}$  and  $\delta t = 4 \cdot 10^{-9}$ . Inside each box, we used a finite difference approximation in space, with mesh width  $\delta x = 1 \cdot 10^{-5}$  and `lsode` as time-stepper. The initial condition is

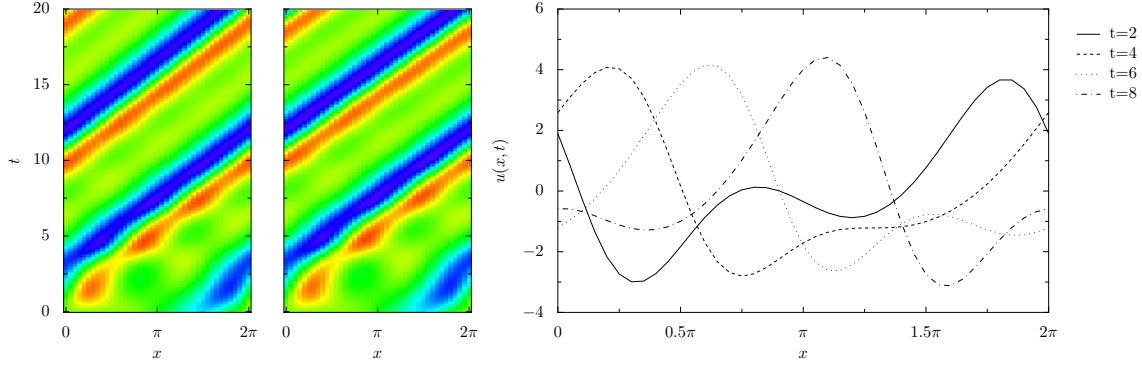


Figure 11: Left: solution of equation (45) using the patch dynamics scheme as a function of space and time. Colors indicate values (blue = 4, red = -4). Right: snapshots of the solution at certain moments in time, clearly showing the approach to a travelling wave solution.

given by

$$u(x, 0) = \begin{cases} -1, & x \in [0, 0.8\pi], \\ -1 + 5(x - 0.8\pi), & x \in [0.8\pi, 1.5\pi], \\ 2.5 - 7(x - 1.5\pi), & x \in [1.5\pi, 2\pi], \end{cases}$$

The results are shown in figure 11. We clearly see both the initial transient and the final travelling wave solution. For comparison purposes, the same computation was performed using the finite difference comparison scheme for the effective equation. Figure 12 shows the errors of the patch dynamics simulation with respect to the finite difference simulation. We see that during the transient phase the error oscillates somewhat, but once the travelling wave is steady the error increases linearly, due to a difference in the approximated propagation speed. Note that the error is significantly larger than for example 5.1, due to the fact that the estimator is less accurate, but also because the macroscopic time-step is much smaller, resulting in a larger number of estimations.

## 6 Conclusions

We described the patch dynamics scheme for multi-scale problems. This scheme approximates an unavailable *effective* equation over macroscopic time and length scales, when only a microscopic evolution law is given; it only uses appropriately initialized simulations of the microscopic model over small subsets (patches) of the space-time domain. Because it is often not possible to impose macroscopically inspired boundary conditions on a microscopic simulation, we propose to use buffer regions around the patches, which temporarily shield the internal region of the patches from boundary artefacts.

We analytically derived an error estimate for a model homogenization problem with

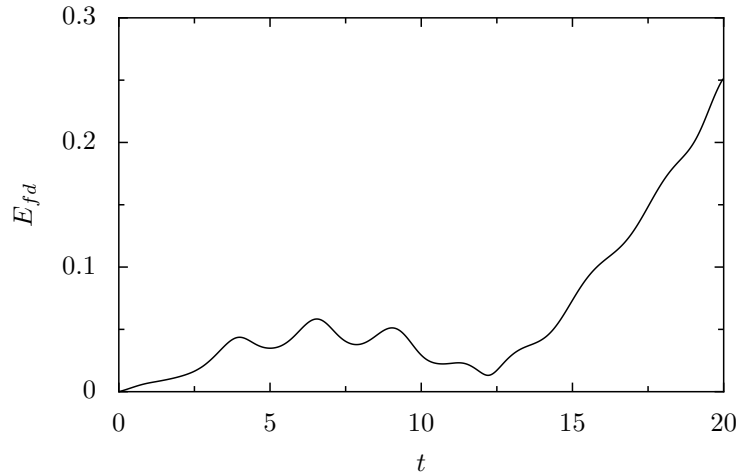


Figure 12: Error of a patch dynamics simulation for equation (45) with respect to the a finite difference comparison scheme for the effective equation. We see that this error grows monotonic once the travelling wave has been reached, due to a slight difference in propagation speed.

Dirichlet boundary conditions. The numerical results show that the algorithm is more widely applicable. We showed the scheme is capable of giving good approximations for reaction-diffusion systems, as well as for fourth order PDEs, such as the Kuramoto–Sivashinsky equation. As such, these results are far more general than those of [29], which are restricted to reaction-diffusion problems due to the special choice of boundary conditions.

We emphasize that, although analyzed for homogenization problems, the real advantage for the methods presented here lies in their applicability for microscopic models that are not PDEs, such as kinetic Monte Carlo, or molecular dynamics. Experiments in this direction are currently being pursued actively.

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