Equation-Free function toolbox for Matlab/Octave: Full Developers 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.

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1 Introduction

Subsubsection contents

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This Developers Manual contains line-by-line descriptions of the code in each function in the toolbox, and each example. For basic descriptions of each function, quick start guides, and some basic examples, see the User Manual.

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

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

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

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

MATLAB appears the obvious choice for a first version since it is widespread, reasonably efficient, supports various parallel modes, and development costs are reasonably low. Further it is built on BLAS and LAPACK so potentially the cache and superscalar CPU are well utilised. Let's develop functions that work for both MATLAB/Octave. Appendix A outlines some details for contributors.

2 Quick start

Section contents

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

2.1 Cheat sheet: Projective Integration

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

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

The cheat sheet consists of two flow charts. Figure 1 overviews constructing a PI simulation. Figure 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, Section 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 3 overviews the chief functions involved and their interactions.

Figure 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.

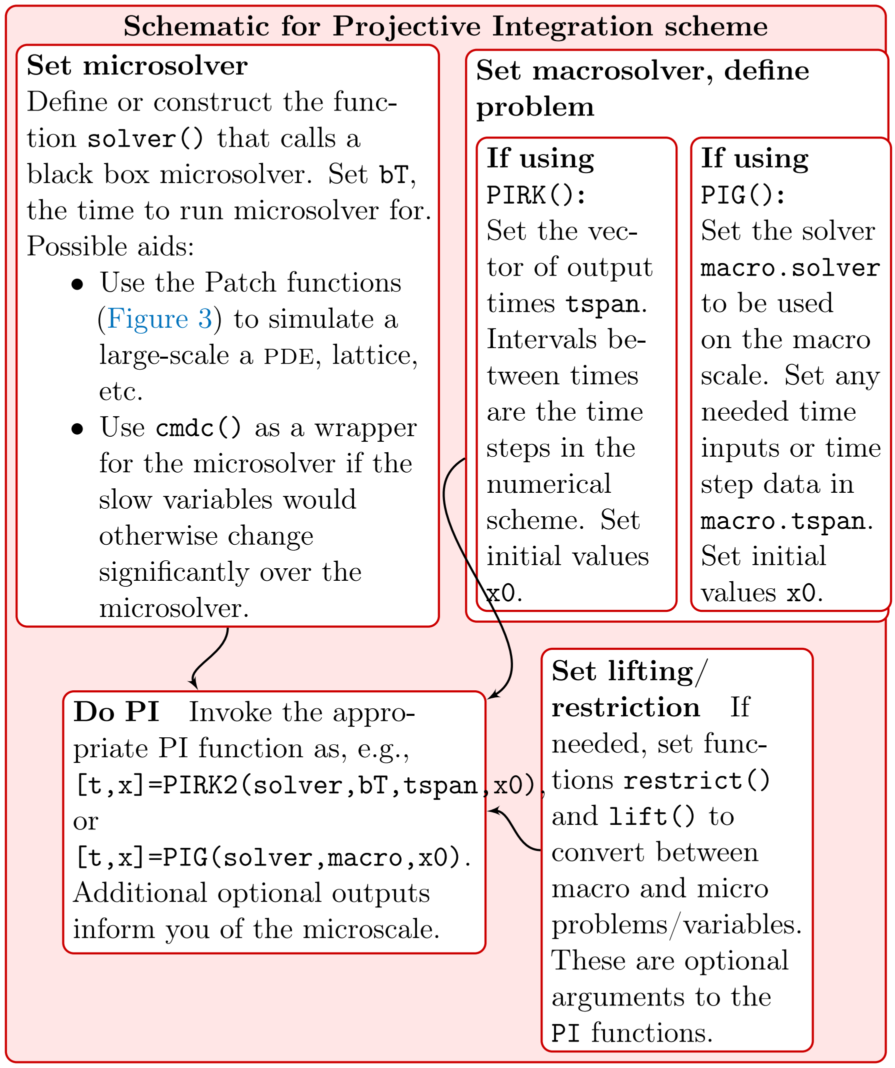


Figure 2

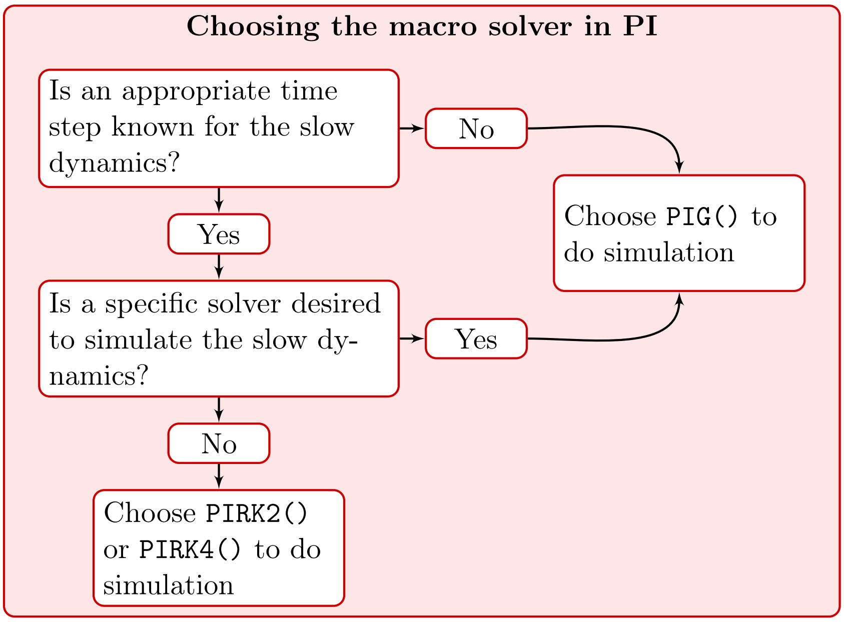
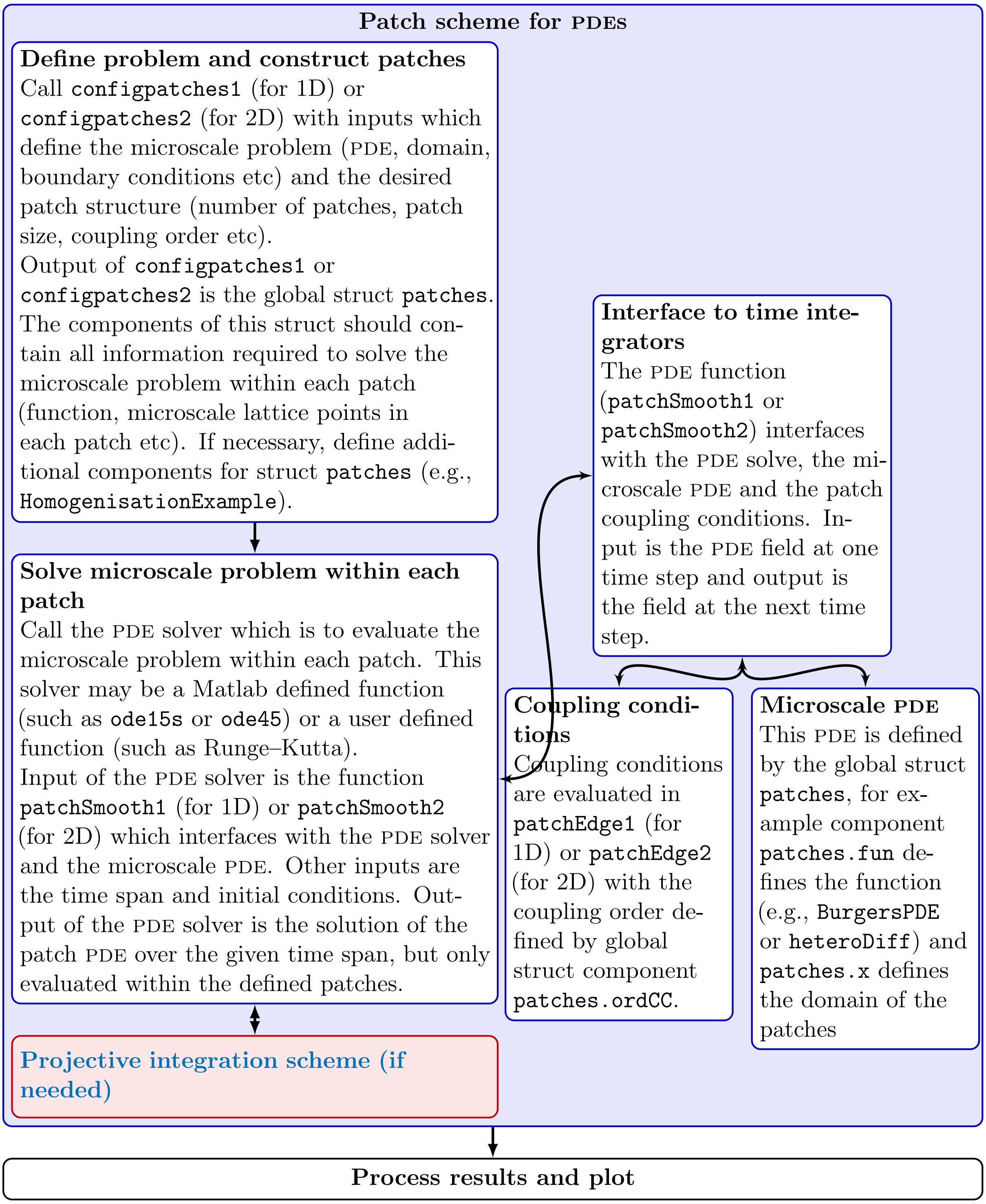

Choosing the macro solver in PI
Is an appropriate time step known for the slow dynamics?
No
Choose PIG() to do simulation
Yes
Is a specific solver desired to simulate the slow dynamics?
Yes
No
Choose PIRK2() or PIRK4() to do simulation

Figure 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

References

Bunder, J., Roberts, A. J. & Kevrekidis, I. G. (2016), 'Accuracy of patch dynamics with mesoscale temporal coupling for efficient massively parallel simulations', *SIAM Journal on Scientific Computing* **38**(4), C335–C371.

Calderon, C. P. (2007), 'Local diffusion models for stochastic reacting systems: estimation issues in equation-free numerics', *Molecular Simulation* **33**(9—10), 713—731.

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

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

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

Gustafsson, B. (1975), 'The convergence rate for difference approximations to mixed initial boundary value problems', *Mathematics of Computation* **29**(10), 396–406.

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

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

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

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

Liu, P., Samaey, G., Gear, C. W. & Kevrekidis, I. G. (2015), 'On the acceleration of spatially distributed agent-based computations: A patch dynamics scheme', *Applied Numerical Mathematics* **92**, 54–69.
http://www.sciencedirect.com/science/article/pii/S0168927414002086

Plimpton, S., Thompson, A., Shan, R., Moore, S., Kohlmeyer, A., Crozier, P. & Stevens, M. (2016), Large-scale atomic/molecular massively parallel simulator, Technical report, http://lammps.sandia.gov.

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

Roberts, A. J. & Li, Z. (2006), 'An accurate and comprehensive model of thin fluid flows with inertia on curved substrates', *J. Fluid Mech.* **553**, 33–73.

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

Samaey, G., Roberts, A. J. & Kevrekidis, I. G. (2010), Equation-free computation: an overview of patch dynamics, *in* J. Fish, ed., 'Multiscale methods: bridging the scales in science and engineering', Oxford University Press, chapter 8, pp. 216–246.

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

Svard, M. & Nordstrom, J. (2006), 'On the order of accuracy for difference approximations of initial-boundary value problems', *Journal of Computational Physics* **218**, 333–352.