Minisymposium 110: Effective multiscale computational modeling of spatio-temporal systems

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Better buffers for patches in macroscale simulation of systems with microscale randomness

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University of Adelaide and Princeton University

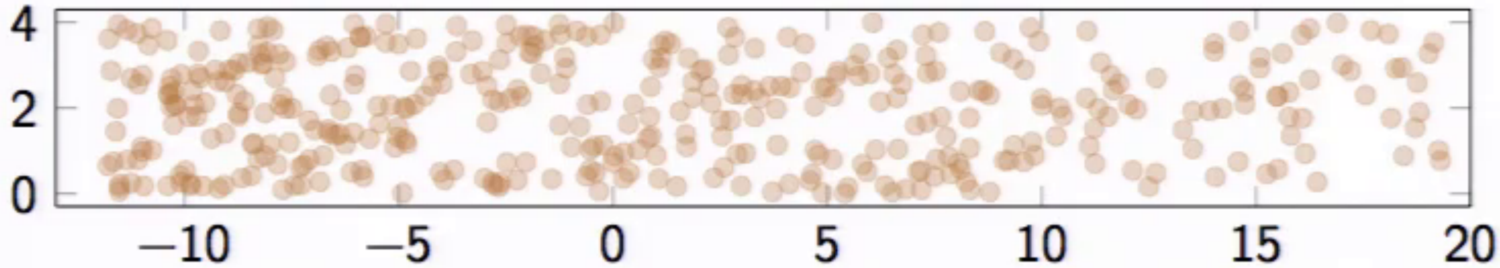
May 20, 2015

[1] Funded by the Australian Research Council

Schematic overview

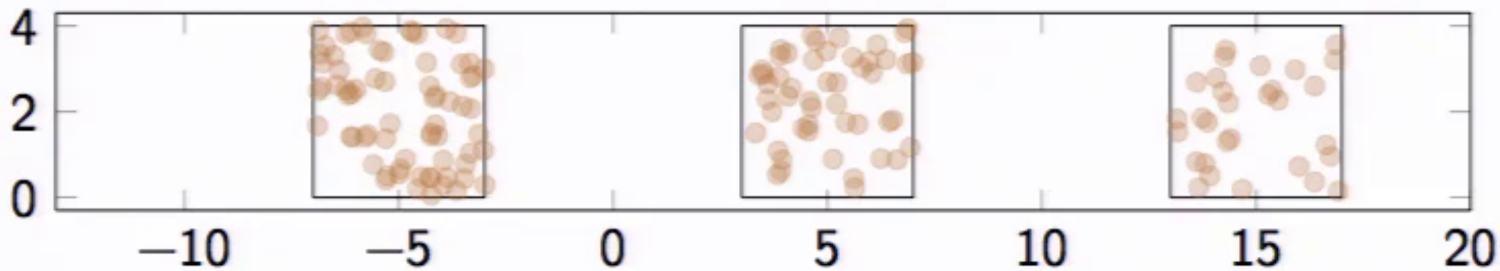
We have an 'atomistic'/'agent' based computational model.

Its computations predict evolution in space-time: *large*.



Assume the computation is far too expensive over desired space domain.

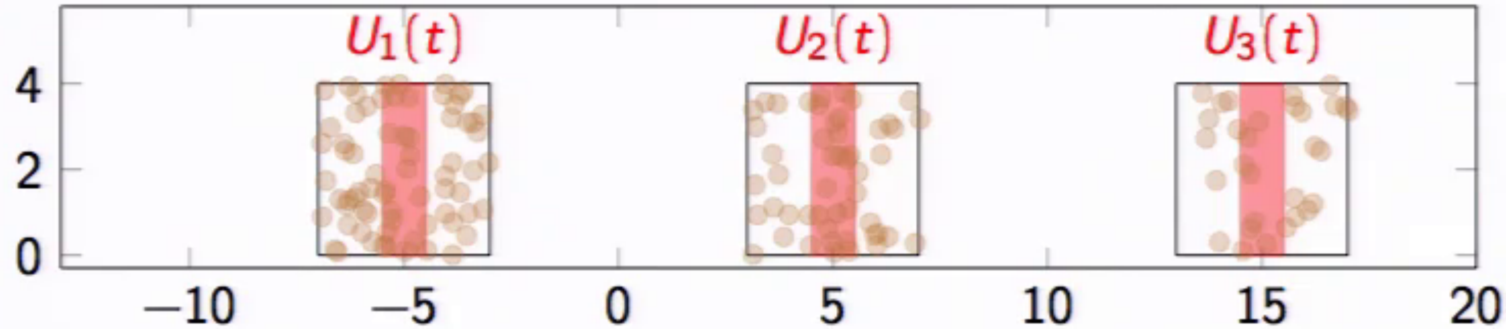
Instead, restrict computation to small microscale patches of space.



How do we couple patches for a coherent macroscale prediction?

To couple, choose macroscale variable, say U

Define macroscale values $U_j(t)$ as average over *core* of jth patch.



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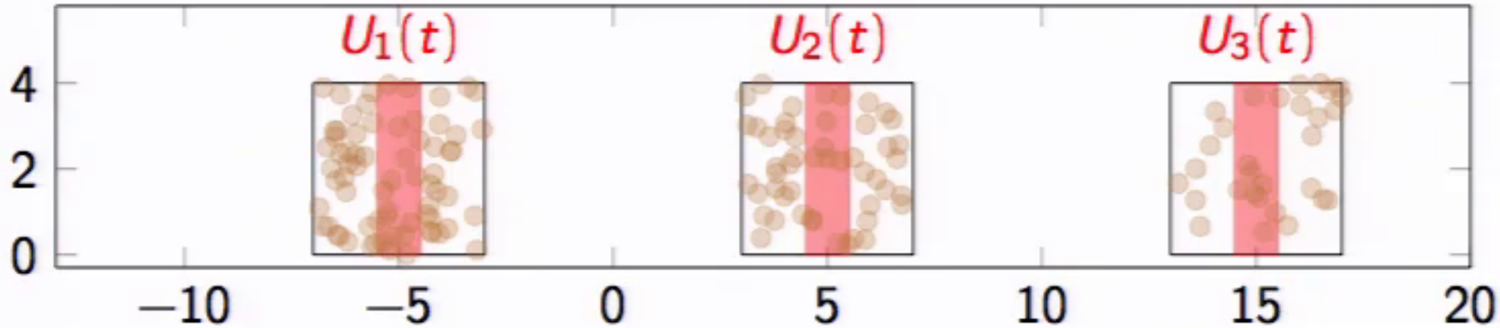
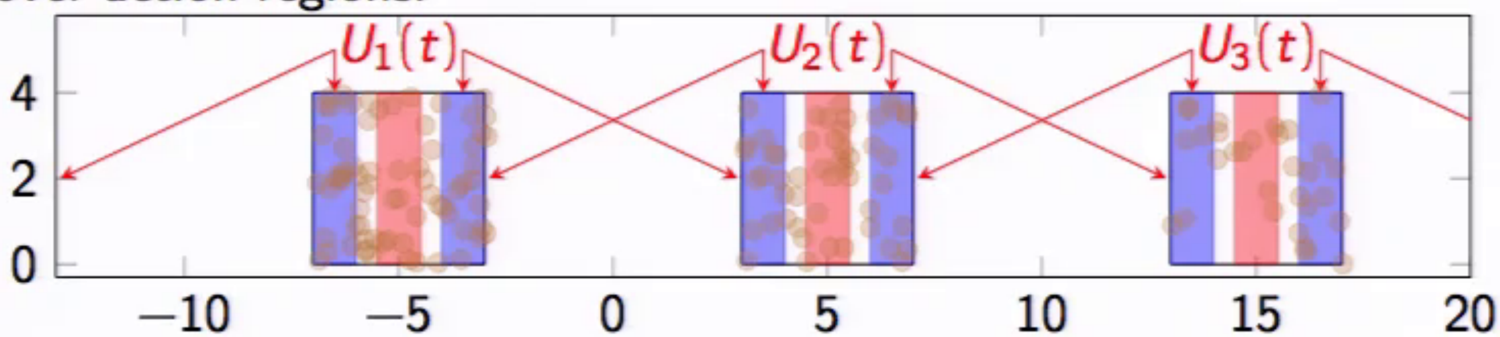


Then couple patches via some interpolation of $\vec{U}(t)$ by applying control over *action* regions.



Challenges: what interpolation? how big are the core and action regions?

Answer for interpolation

If the macroscale variable(s) chosen correctly, then there exists a sound smooth macroscale closure for field $U(x,t)$:

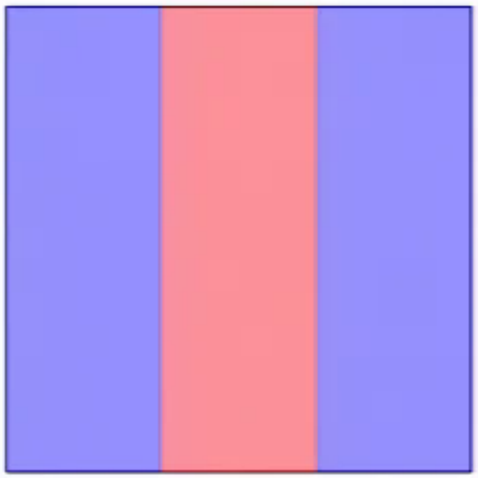
$$U_t = F(U, U_x, U_{xx}, \ldots).$$

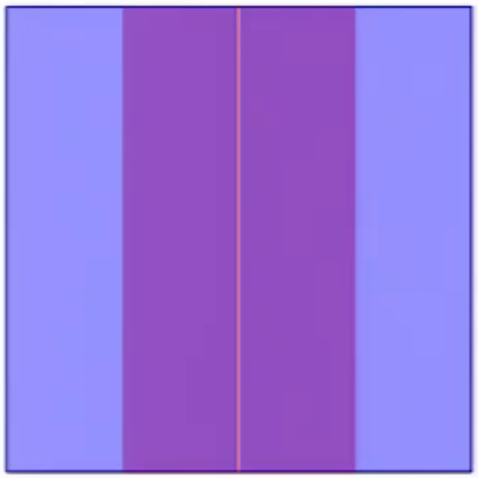
For such an in-principle closure, previous research established classic Lagrangian interpolation is good: $\mathcal{O}(H^p)$ in patch spacing H.

- A. J. Roberts and I. G. Kevrekidis. General tooth boundary conditions for equation free modelling. *SIAM J. Scientific Computing*, 29(4):1495–1510, 2007.
- M. Cao and A. J. Roberts. Multiscale modelling couples patches of non-linear wave-like simulations. [http://http://arxiv.org/abs/1404.6317], 2014.

Propose answer for core and action regions

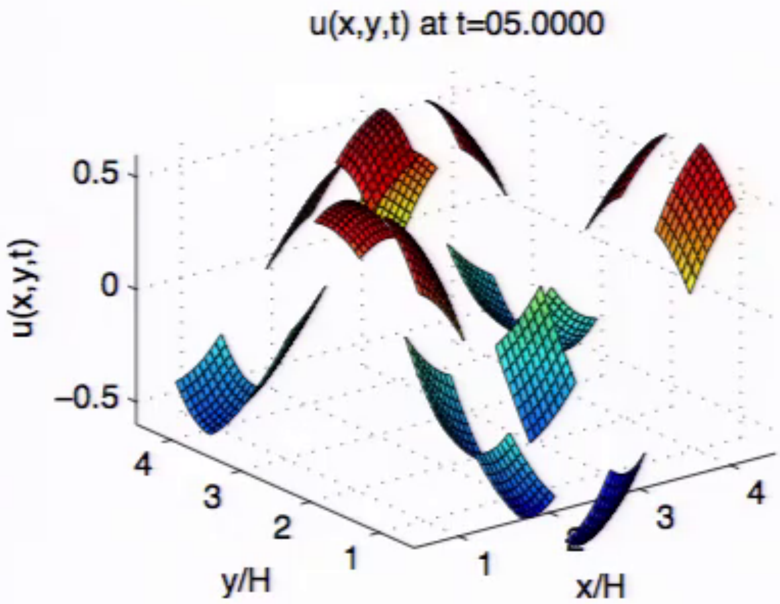
Make each of the cores and action regions from a third to a half of their patch.

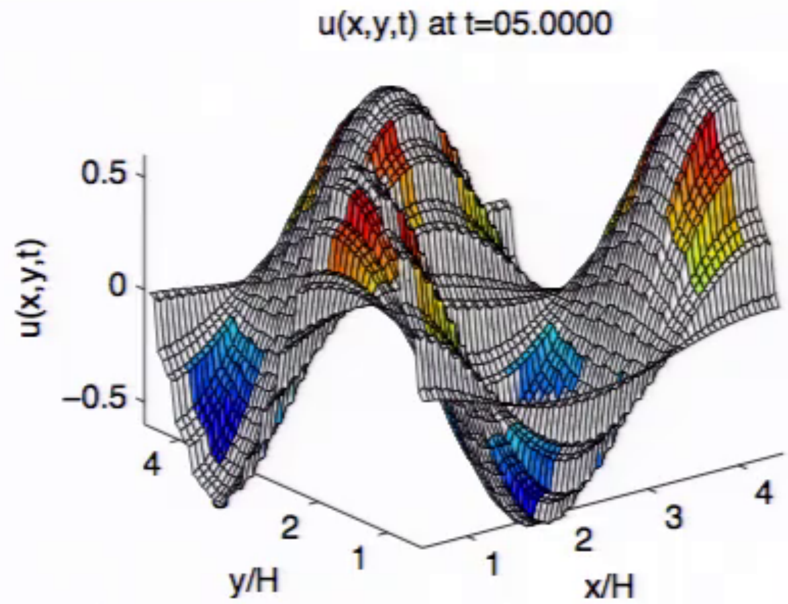




The best buffer is none at all!

Discuss 1D, but multi-D appears OK





Simulations of 2D lattice diffusion with varying microscale diffusivity: (left) ensemble average of $u(x, y, t)$ for patch dynamics; and (right) $u(x, y, t)$ simulated on all space for one diffusivity realisation (colours marking the patches used in the left scheme).

Homogenise microscale varying 1D diffusion

Why? Mesoscale diffusion is emergent from a wide variety of microscale problems. We can and do fully analyse microscale diffusion.

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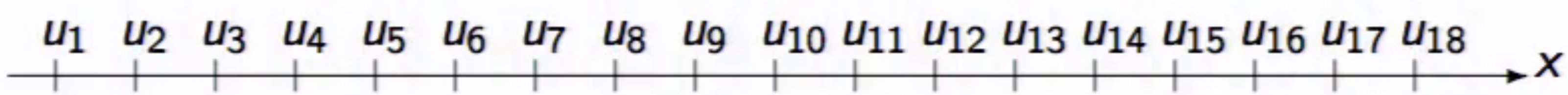
Consider diffusion for the field $u_i(t)$ on a 1D micro-lattice:

$$\dot{u}_i = du_i/dt = \kappa_{i+1/2}(u_{i+1} - u_i)/h^2 + \kappa_{i-1/2}(u_{i-1} - u_i)/h^2 \qquad (1)$$

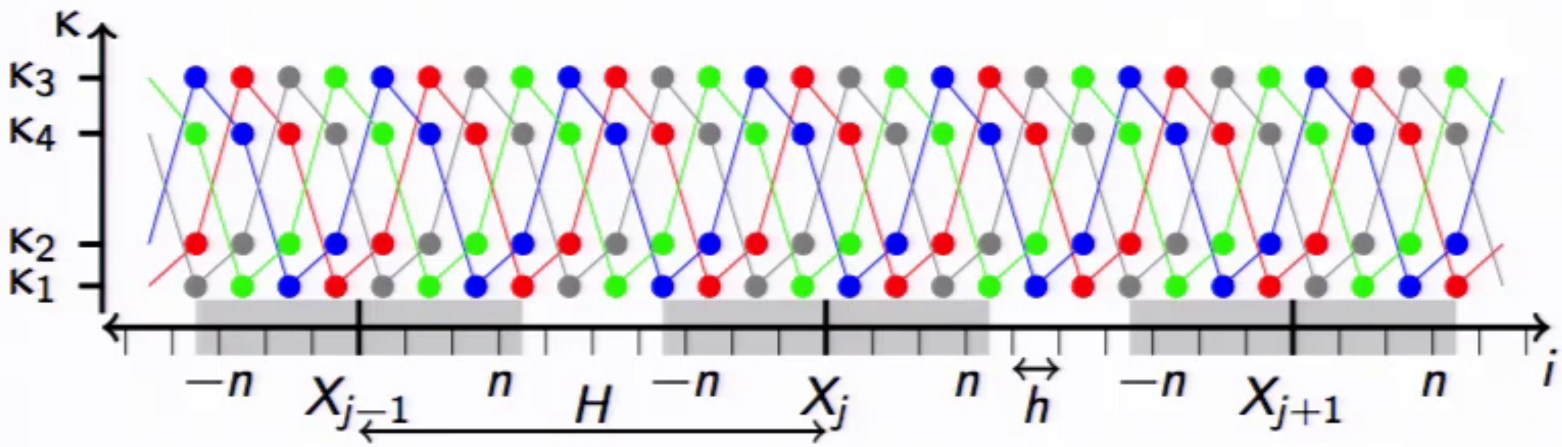
where diffusivities κ_i cycle through K values (K-periodic).



Analyse ensemble average predictions

Expect the phase of the microscale diffusivities is unknown, so analyse ensemble average over different configurations of microscale.

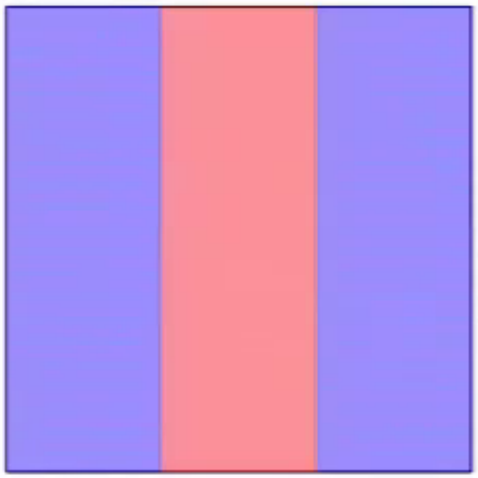
The microscale lattice has spacing h. The macroscale lattice has spacing H. The jth patch of width $(2n+1)h$ about the macroscale lattice point X_j, indicated by the shaded rectangles.

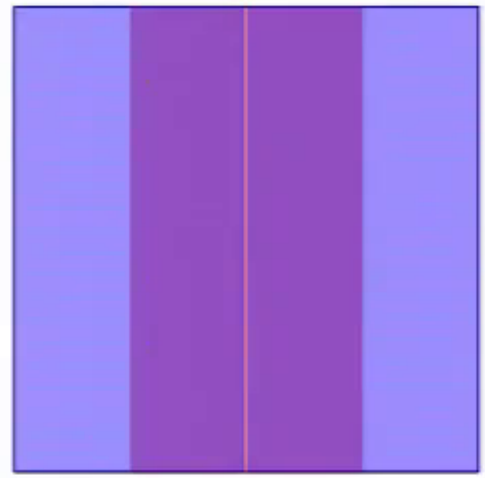


For example of $(K = 4)$-periodic diffusivities, the ensemble contains $2K = 8$ configurations: the four with translation symmetry are illustrated; the remaining are reflections.

Propose answer for core and action regions

Make each of the cores and action regions from a third to a half of their patch.





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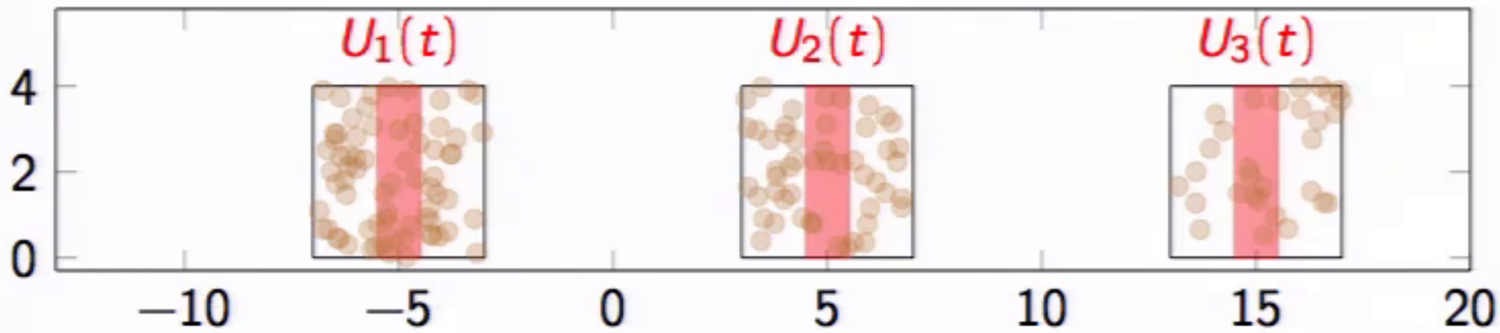

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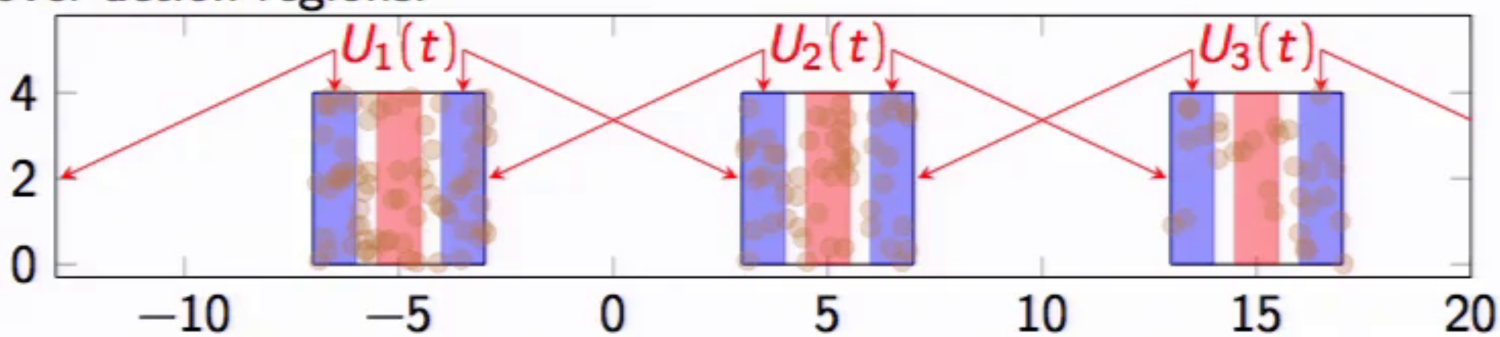

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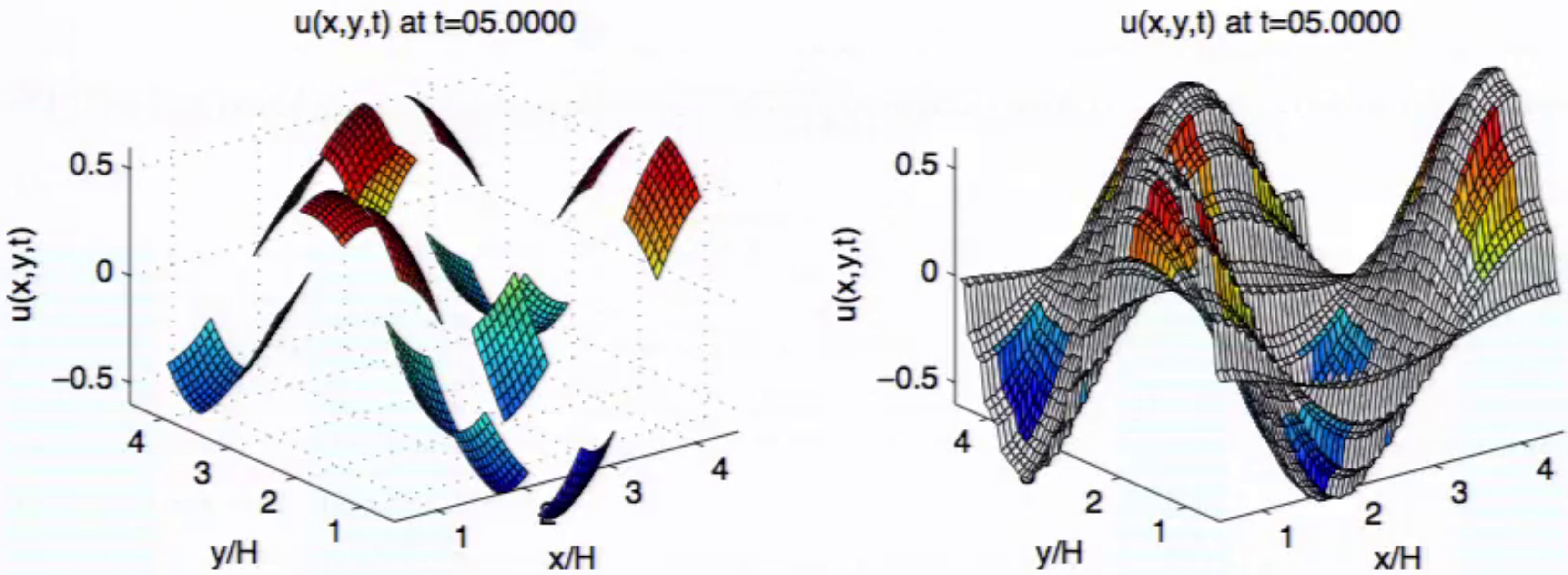

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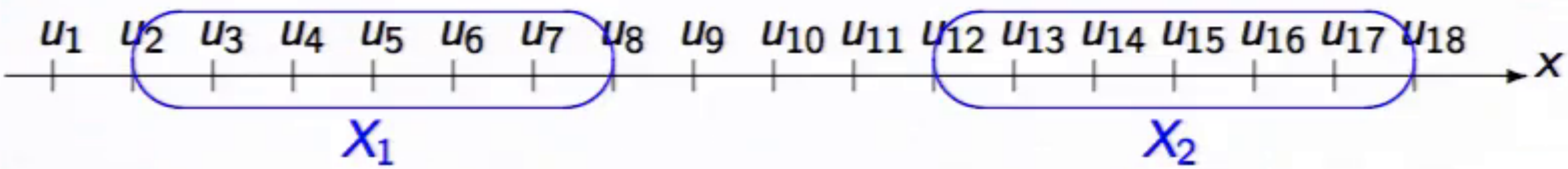

Model by $U_j(t)$ on a macroscale grid X_j of large spacing H by only simulating on microscale patches.

Challenge: couple patches when microscale diffusivity fluctuates?

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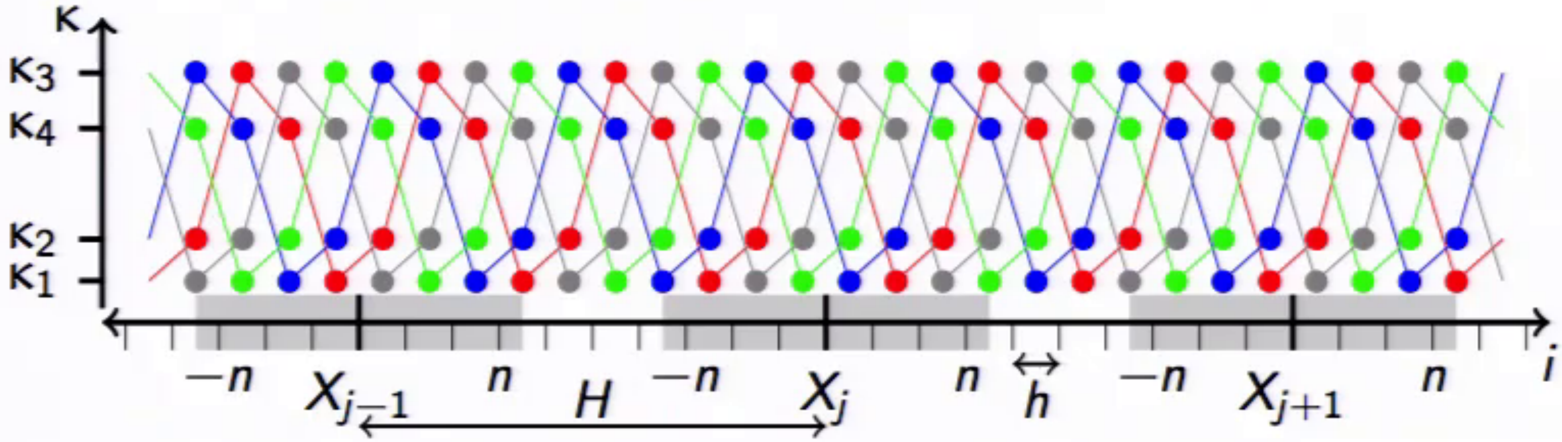

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Full microscale emergent dynamics is the reference

Linear analysis gives slow emergent dynamics on the macroscale as

$$\dot{U}_j = \frac{\kappa}{h^2}\left[\delta^2 + \left(\frac{K^2-1}{12} - \frac{c_2(\vec\kappa)\kappa^2}{K^2\kappa_g^K}\right)\delta^4\right]U_j + \mathcal{O}(\delta^6)\,. \qquad (2)$$

where κ is harmonic average diffusivity (well-established),

$$\kappa_g^K = \prod_{i=1}^{K}\kappa_i\,, \quad \text{and } c_2(\vec\kappa) = \frac{\kappa_g^K}{2}\sum_{m_1=1}^{K}\sum_{m_2=1}^{K-1}\frac{m_2(K-m_2)}{\kappa_{m_1}\kappa_{m_1+m_2}}\,,$$

depends upon the ordering.

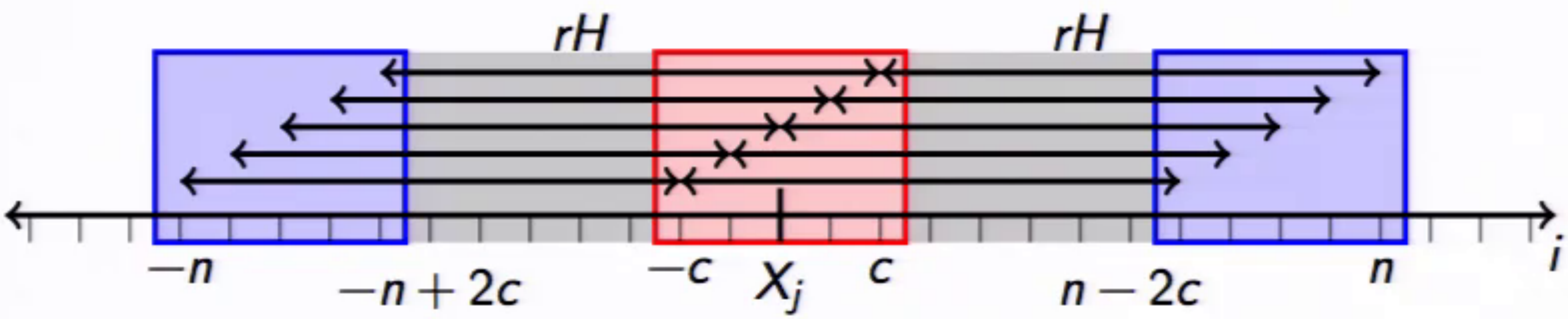
This result follows by writing $d\vec{u}/dt = M\vec{u}/h^2$ for a $K\times K$ operator matrix representing both a period and the operator coupling with neighbouring periods. The 'smallest' eigenvalue of M, of its K eigenvalues, gives (2).

Patch dynamics: core and coupling

Adjoin to microscale lattice equation (1) the macroscale

$$U_j(t) = U(X_j, t) = \left\langle \sum_{i=-c}^{c} \frac{u_{j,i,e}}{2c+1} \right\rangle, \qquad (3)$$

where angle brackets represent ensemble average over all configurations e, and integer c is the core half-width.



In terms of microscale shift operator ε, Lagrangian coupling is

$$\varepsilon^{\pm(n-c)} U_j = \left\langle \sum_{i=n-2c}^{n} \frac{u_{j,\pm i,e}}{2c+1} \right\rangle. \qquad (4)$$

Patch dynamics: evolution

Lattice equation (1), core average (3), and coupling (4) form a closed system for the patch simulation of diffusion with microscale heterogeneities.

Consistency: obtain various orders of accuracy in the macroscale spacing H by truncating the expansion of the coupling term $\varepsilon^{\pm(n-c)}U_j$ to interactions with the nearest Γ neighbours.

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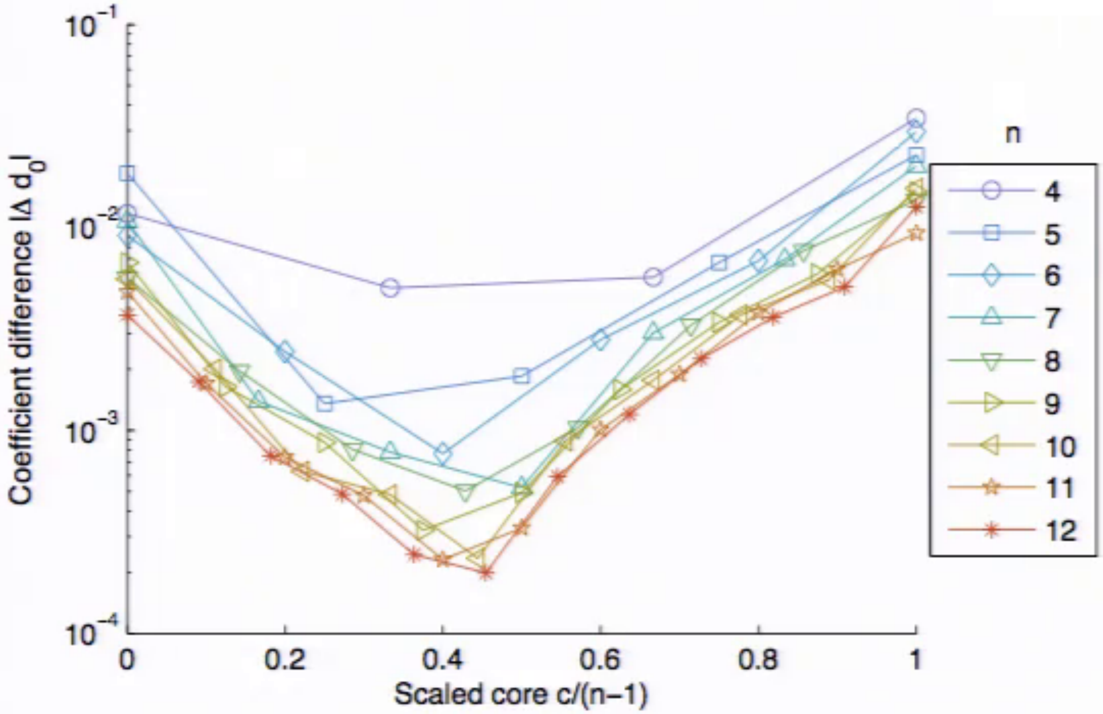
Patch design The emergent slow dynamics of the patch scheme is also findable as $d\vec{U}/dt = \lambda_0\vec{U}/h^2$ for some operator λ_0 that depends upon Γ, $\vec{\kappa}$, the ratio $r = h/H$, and the patch design n and c.

Errors: the error in the patch scheme is the difference between the leading part of λ_0 and the corresponding part of the exact (2).

Patch dynamics: error depends upon design



Error in the leading coefficient averaged over diffusivities $2 \leqslant K \leqslant n$ relative to the scaled core half-width $0 \leqslant c/(n-1) \leqslant 1$ for $4 \leqslant n \leqslant 12$.

The coefficient error is minimised when $c \approx n/2$.

For diffusivity periods $K > n$ (patch half-width) the error is larger $\Longrightarrow$ patches should cover at least two periods of microscale variation.

Mesoscale temporal coupling for parallel computing

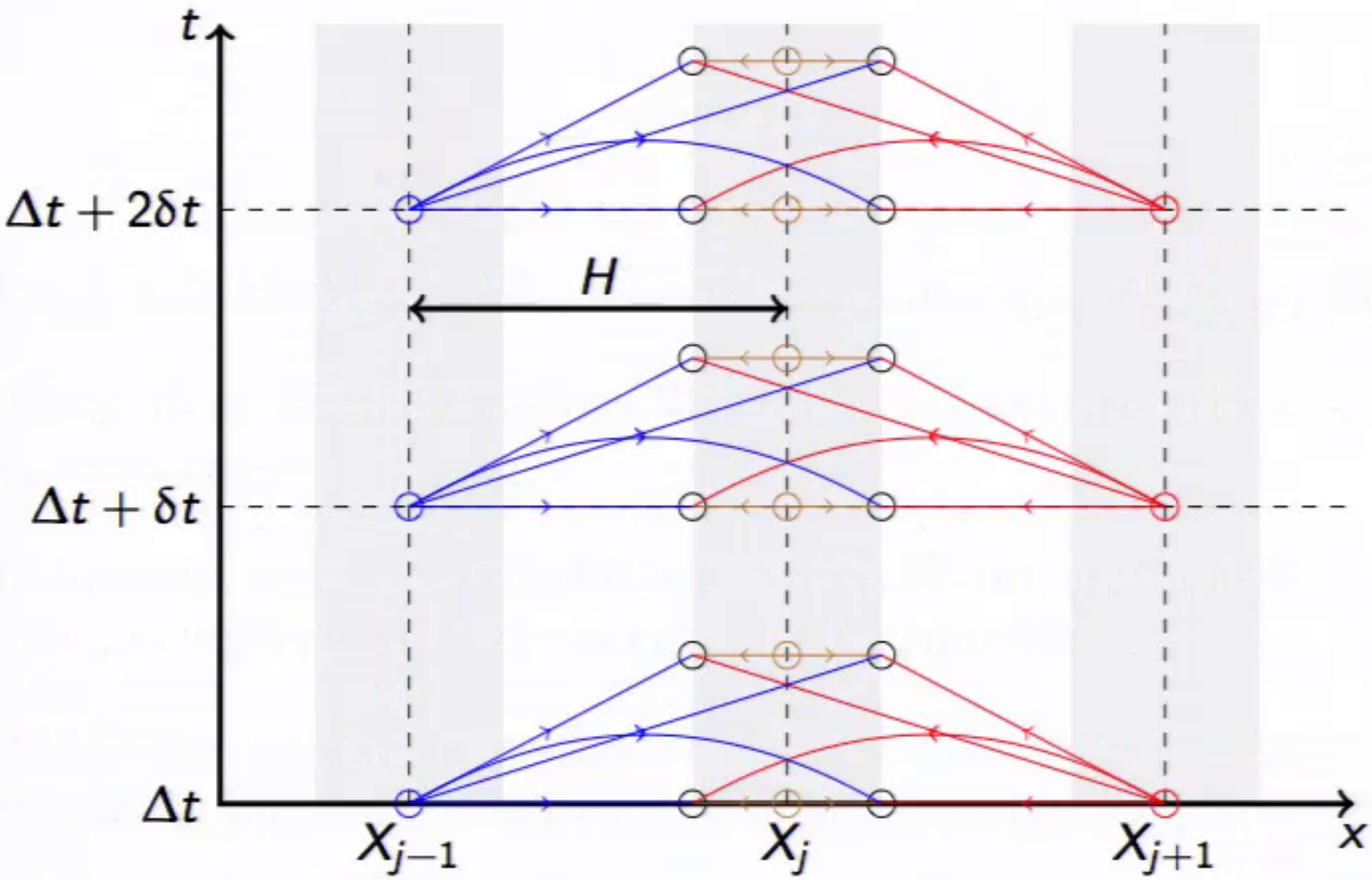
Largest simulations will require multi-processor parallel computing.

The performance limitation will then be communication between processors.

If one processor is assigned to one patch, then the required communication is just the coupling between patches.

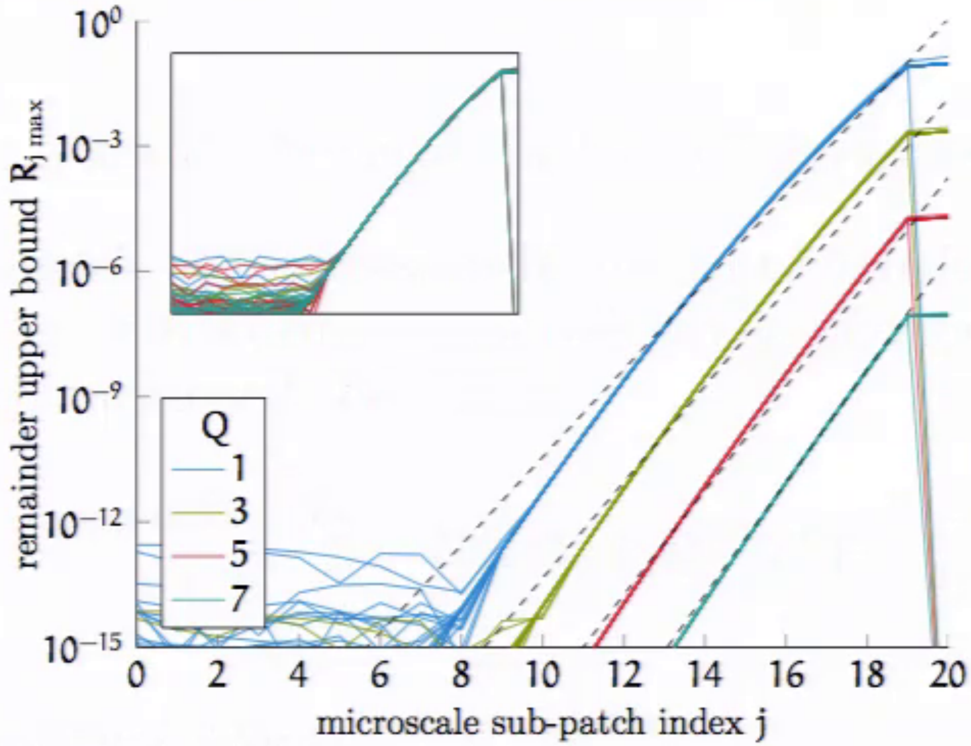
Challenge To reduce communication delays, can we only communicate coupling at mesoscale time intervals (instead of each microscale step)?

Mesoscale coupling



Schematic of the coupling conditions (5) for the jth patch with nearest neighbour coupling where coupling values between patches is only evaluated and communicated at mesoscale time steps δt. As indicated, the average (3) on patches $j \pm 1$ and j feed into the coupling conditions (5) on the jth patch.

Incurred error: distribution across a patch



The solid lines describe the upper bound of components of the error in a patch with half-width $n = 20$, $\cos\ell = 0.91$, mesoscale time $\delta t = 0.5$ and number of f derivatives $Q = 1, 3, 5, 7$. Lines with the same colour have the same Q but all possible core half-widths $c = 0, \ldots, 19$ (insignificant differences). Inset: the error on the same scale as the main plot with $n = 20$, $\delta t = 0.5$, $Q = 1$, and different patch widths.