GreenPhysECS: Exploring ECS for Energy-Aware Parallel Research Software

Oluwole Delano, Mattias Evans, Michael Sparks*
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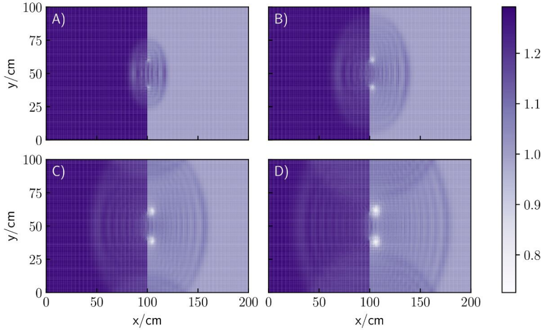

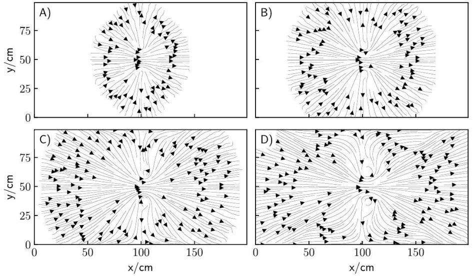

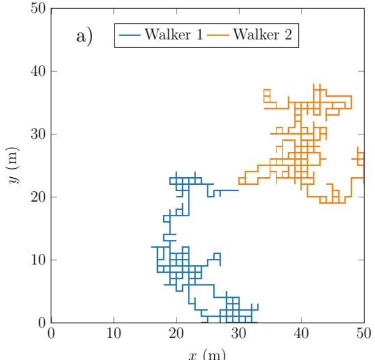

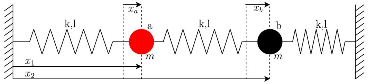

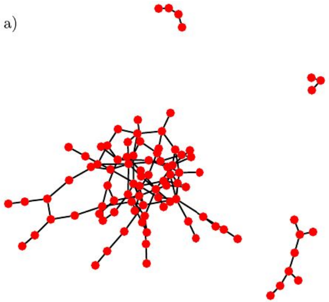

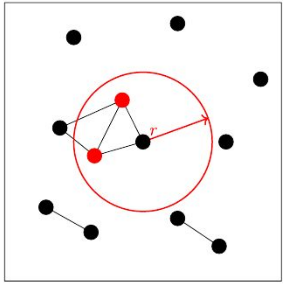

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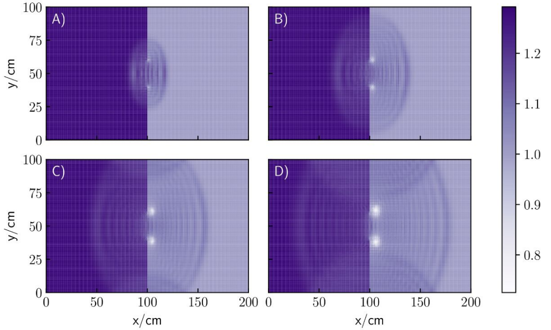

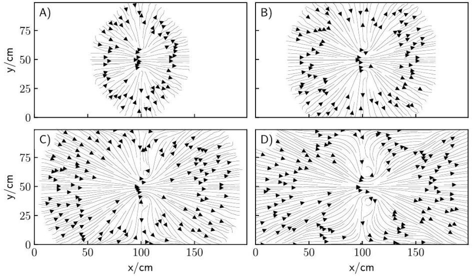

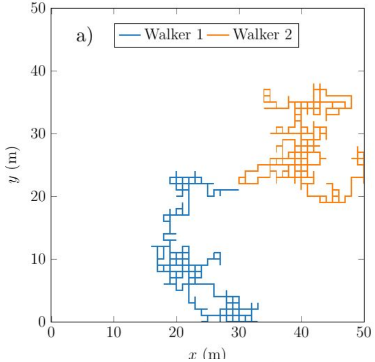

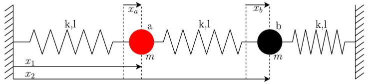

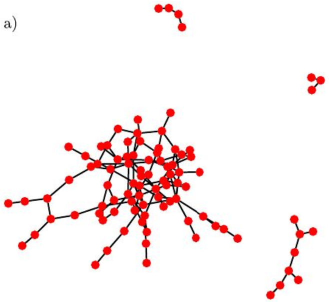

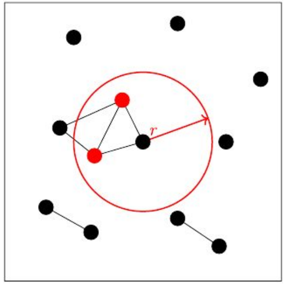

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Problem

- Physics Workloads are embarrassingly parallel
- Highly parallel hardware is now standard - **from laptops through clusters**

- **Software pedagogy, practice and tooling often remain linear - which does not map well onto such infrastructure**

- **Valuable research infrastructure can remain difficult to use effectively - especially for ECRs**

The problem is fundamentally around **enabling and widening good utilisation** of modern infrastructure

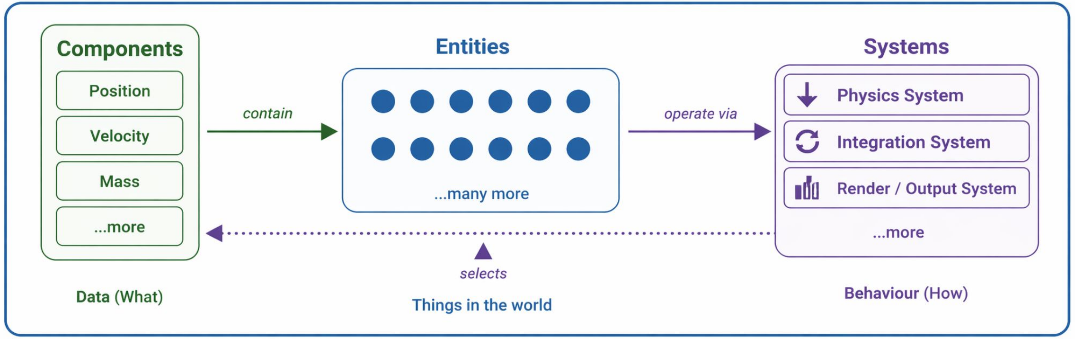
(for ECRs and others)

Entity Component Systems - ECS

- **Widely used in media** for data parallel simulation (film, SFX, games)
- **Separates data from behaviour.**
- Entities contain components.
- **Systems operate a single transform across many entities - highly parallel**
- Systems are highly focussed, helping with processor cache coherency at scale.

- Inspired by physics
- **Rarely used outside media**
- AtomECS (Cambridge) notable exception

GreenPhysECS - explores ECS utility for ECRs to build scalable research software



Constraints & Tooling

Technical Overview

- C++20 codebase
- Flecs as the ECS library
- RAPL-based energy tracking library
- Docker for consistent cross builds

Multicore & GPU deferred due to timing constraints - BUT the code is naturally concurrent.

Practical Constraints

- Project undertaken by MPhys students
- Each project was 1 semester long, approx 2 days/week
- Steep learning curve (low C++ knowledge)
- Laptop based development and simulation
  - Consequences for energy tracking testing and diversity of tested platforms

Benefits:

- Reproducible builds across Mac, Windows, Linux
  - https://github.com/UofM-Green-Compute/GreenPhysECS
- Can't get any earlier ECR than MPhys!
- Focus on practicality over perfection

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The projects

Testing this hypothesis requires real work

- Fluid Dynamics
- Epidemiology - general and mitigations for outbreaks in crops

A flavour of this work follows - GreenPhysECS is extracted from this work

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Project 1: Fluid Dynamics

Project 1: Fluid Dynamics

- Computational Fluid Dynamics is a well developed field
- Different numerical techniques exist
  - Can explore different utility of ECS in different cases
- Two techniques were considered:
  - Finite Difference Method
  - Smoothed Particle Hydrodynamics

Two approaches: Eulerian and Lagrangian

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Eulerian

- Fixed positions
- More matrix and/or differential equations based

Lagrangian

- Fixed parcels of fluid flow
- More dynamics based

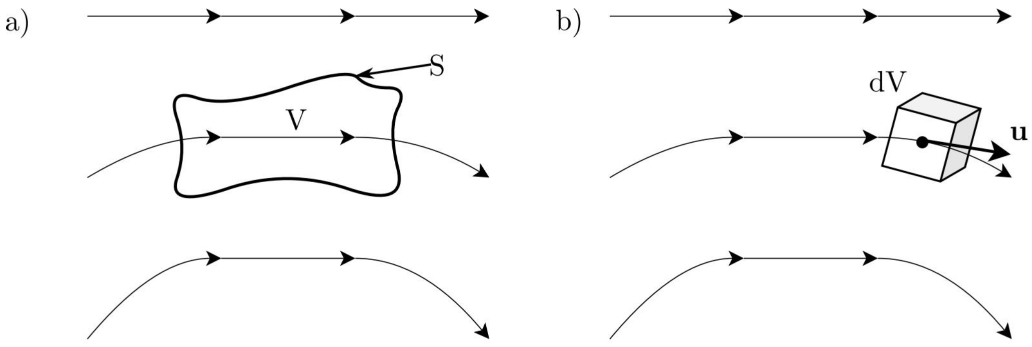

Figure 2: Diagram showing the a) the Eulerian picture of a fluid flow, and b) the Lagrangian picture of a fluid flow

Finite Difference Method (FDM)

- The FDM approximates a continuous domain by a set of discrete points
- Derivatives can then be approximated by considering the value of a function at neighbouring points

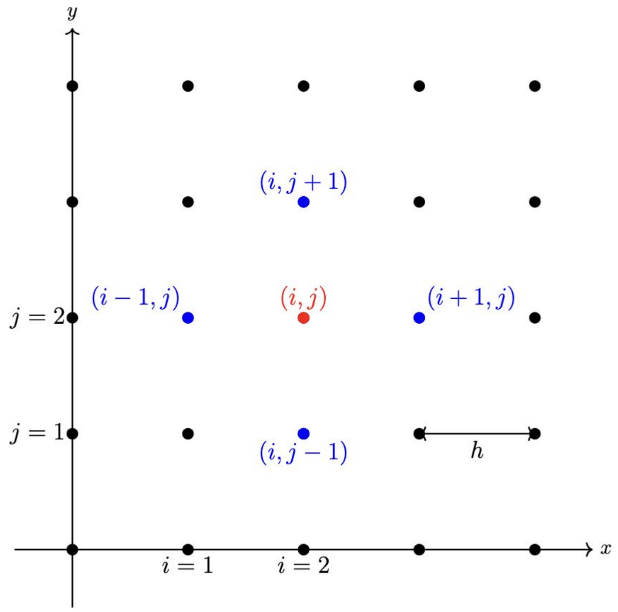

Figure 3: Figure showing a two dimensional cartesian mesh.

Smoothed Particle Hydrodynamics (SPH)

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- Smoothed particle hydrodynamics (SPH) is a lagrangian approach to simulating a fluid
- The approach relies on approximating the macroscopic properties of a fluid (pressure, density, etc) based on the distribution of the fluid elements
- This reduces to an equation of motion for each particle (essentially F = ma)

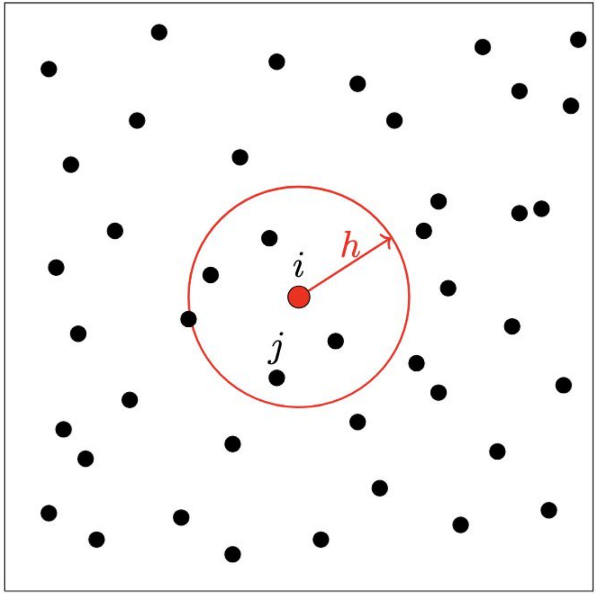

Figure 4: Figure showing SPH particles in a box. The radius around each particle represents the smoothing radius around each particle.

Smoothed Particle Hydrodynamics (SPH)

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- Approximate a function based on a knows distribution of fluid elements
- Particles within some radius, h, of each other are summed over to estimate the value of a property (e.g. density)
- An interpolation function is used to weight this sum
- $$\rho(r) = \sum_b m_b W(r - r_b, h)$$

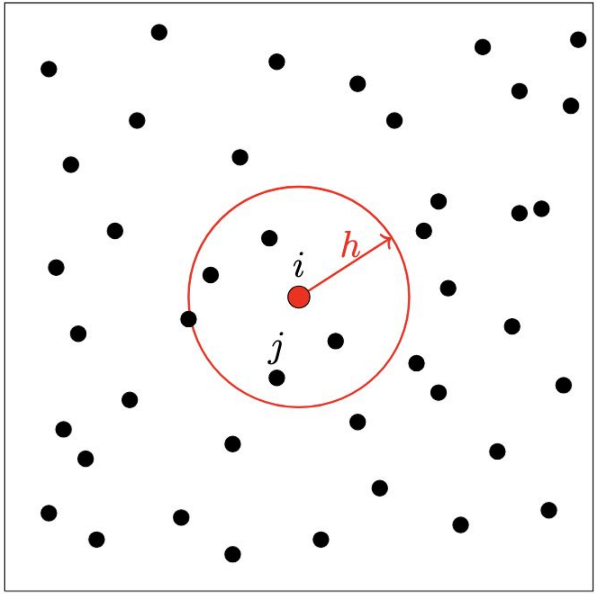

Figure 4: Figure showing SPH particles in a box. The radius around each particle represents the smoothing radius around each particle.

Implementation - Fluid in a box

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FDM:

- Each point in the grid was an entity
- At each point the position, velocity, density, were components
- Systems evolve according to the discretized euler equations

SPH:

- Entities were particles of the fluid
- Components were the position, velocity, and acceleration
- Systems were used to implement collisions and evolve the components of the particle according the the equation of motion

Fluid Dynamics Results

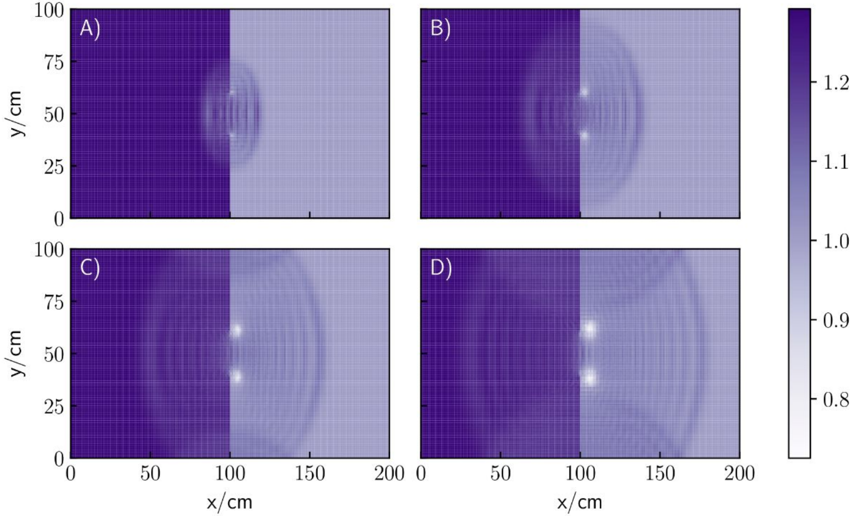

Figure 5: Graphs showing the evolution of the density plot (FDM). The graphs are evaluated at times A) t = 0.001s, B) t = 0.002, C) t = 0.003s, and D) t = 0.004s.

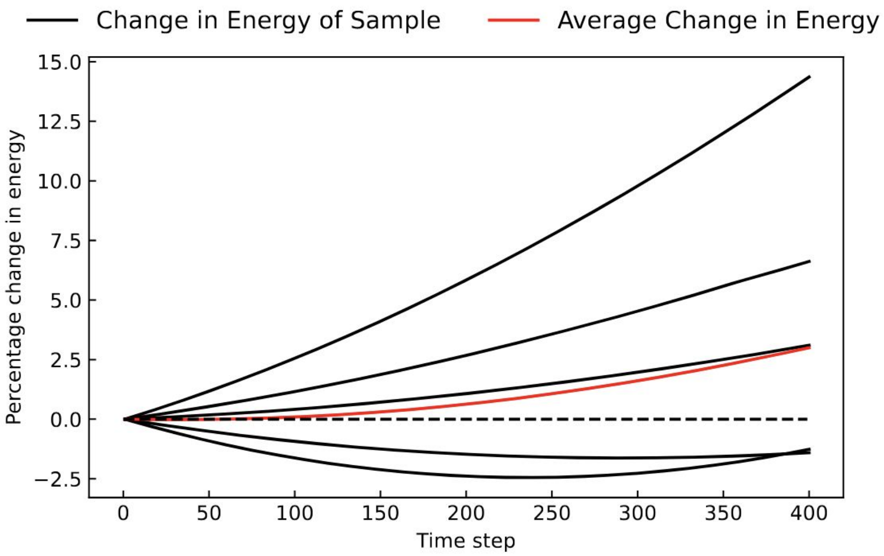

Figure 6: Change in total energy of the system for a time step t = 0.000001

Energy Tracking

- **Energy tracking was implemented** during this phase of work
- This uses an API **using RAPL** measurements and CodeCarbon but for C++
- This is implemented **as an extra SYSTEM** that runs alongside the other systems
- **This allows "book-ending" others system** for measurement
- That means the energy tracking can be dropped into any ECS based simulation easily

This serves as a good proof of principle and needs extra work

Fluid Dynamics Takeaways

Pros

- **ECS shines most where many small entities with similar properties can be created**
- **ECS also shines where the system is active and dynamic**
- **ECS could deal with time-dependent fixed-position differential equations**
    - Not entirely intuitive

Cons:

- ECS was less suited to solving matrix problems - conventional methods are the more natural choice here.

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Project 2: Markov Processes

Markov Processes

- Memoryless stochastic processes
- Widely applicable
- Multiple approaches
  - Matrices
  - Calculus
  - Algorithms

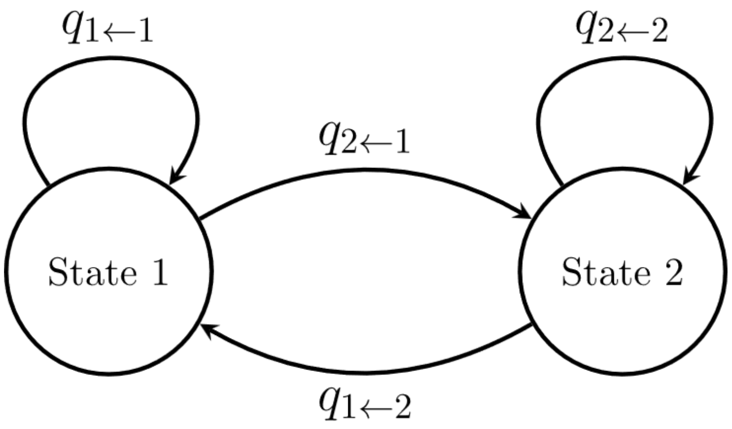

Figure 7: 2-State Markov Chain Diagram

Discrete Time Method

Transition elements:

- $q_{n\leftarrow m} = P(X(t+\Delta t)=n \,|X(t)=m)$
- Δt: time step

1. Set an initial state n=n(0)
2. Determine all possible transitions and their transition elements
3. Draw a random number between 0 and 1 and consequently choose a transition
4. Advance the simulation by Δt
5. Return to step 2

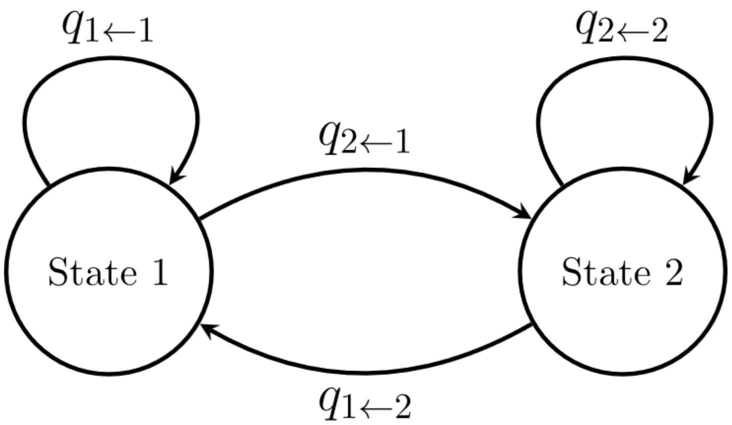

Figure 7: 2-State Markov Chain Diagram

Disease Outbreak Modelling: SIR

- Basic model: SIR model
- Each individual can be in one of three states:
  - S - Susceptible
  - I - Infected
  - R - Recovered

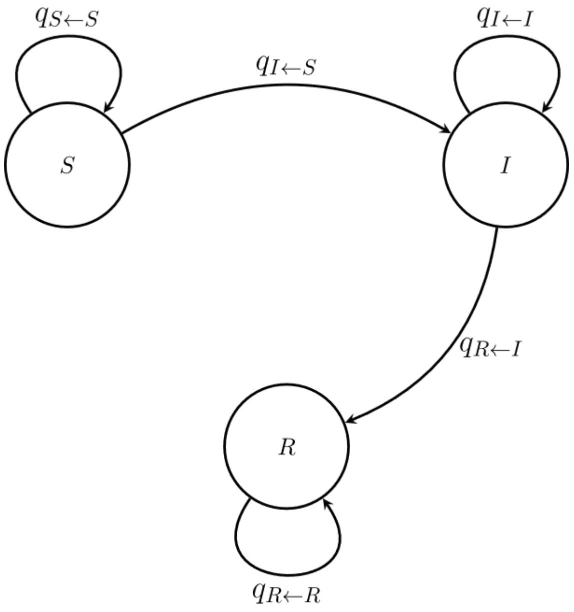

Figure 8: SIR Markov Chain Diagram

Disease Outbreak Modelling: SIR

- Transition Rates
  - $q_{s \to I} = \beta n_I \Delta t$
  - $q_{I \to R} = \gamma \Delta t$
- β: Infection rate
- γ: Recovery rate

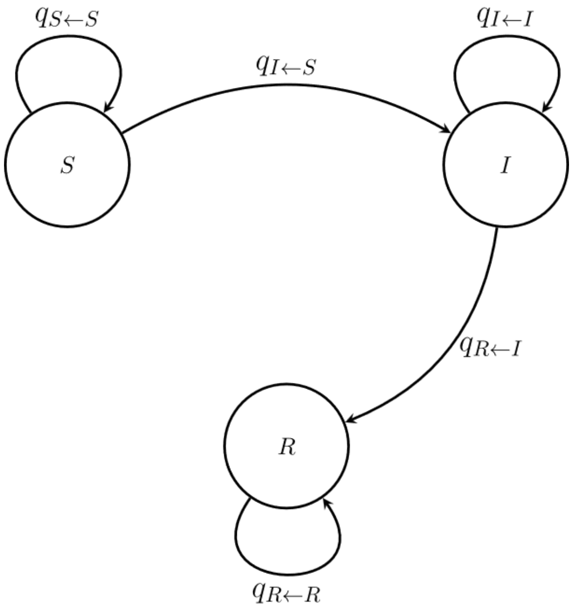

Figure 8: SIR Markov Chain Diagram

Disease Outbreak Modelling: ECS

- Entities:
  - Members of the population
- Components:
  - State
  - Index
  - Transition Probabilities
- Systems:
  - Update Transition Probabilities
  - Update State

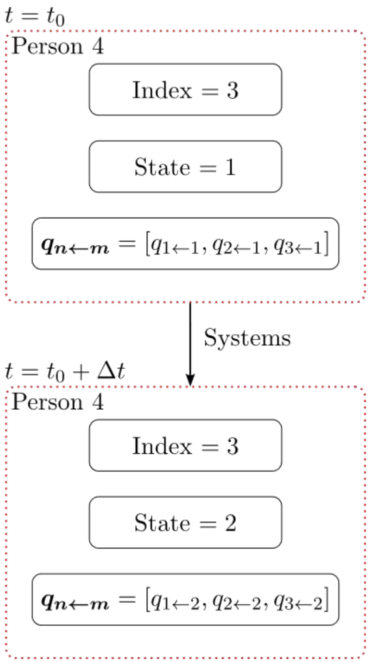

Figure 9: Systems updating the components of an entity

Disease Outbreak Modelling: SIR Results

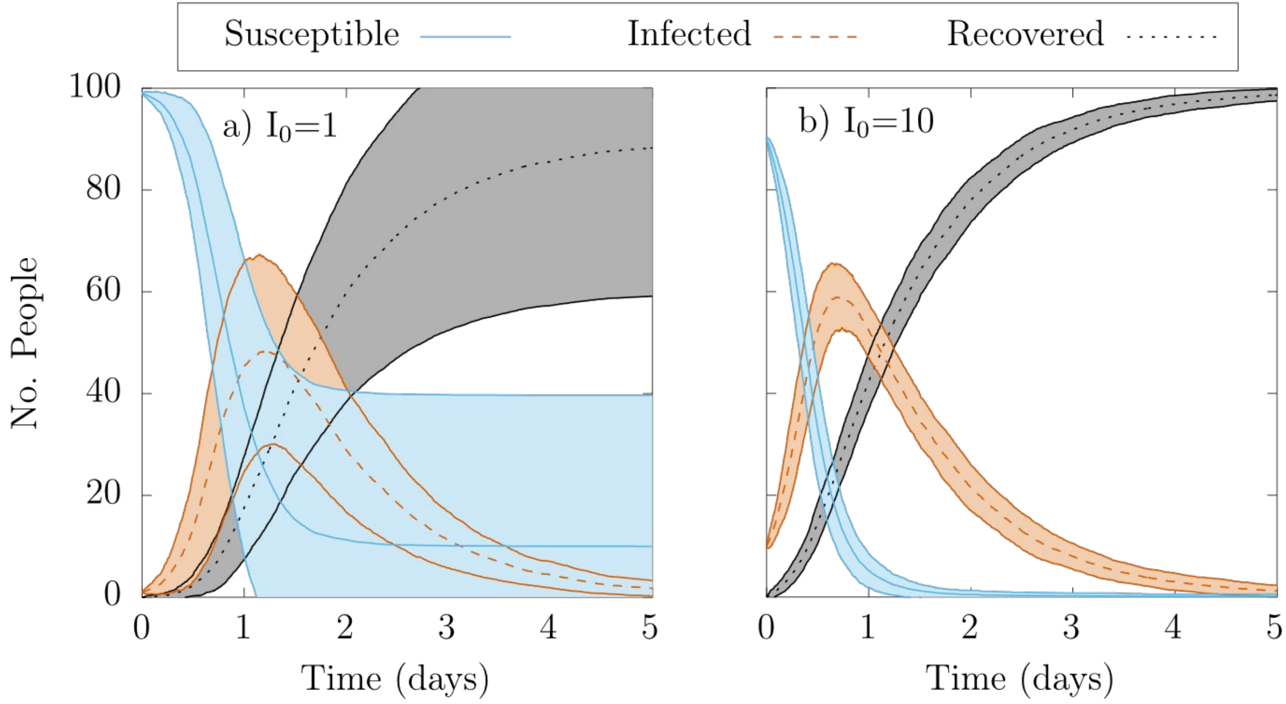

Figure 10: Ensemble averaged SIR model. □ = 7/N where N=100 is the total population γ=1. a) There is initially one infected member of the population. b) There are initially 10 infected members of the population

Disease Outbreak Modelling: Further Work

- Different Compartmental models
  - Eg SEIR
- Network Models
- Spatial Models
  - In particular a spatial Healthy-Undetectable-Detectable (HUD) model for plant epidemics

Disease Outbreak Modelling: ECS Takeaways

- ECS is well suited to epidemic modelling where many entities are involved
- Extension of existing epidemiological models is simple to implement in ECS

Conclusions

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Conclusions and Future

Conclusions

- Early results suggest ECS is useful for ECRs
- Code is naturally concurrent, lending itself to parallel optimisation
- Went beyond the literature surveyed - represents new results in the field

Open Questions

- Does the approach generalise?
- Which problems suit ECS best? (beyond fluid dynamics, epidemiology, etc)
- Can energy awareness become normal practice?

- Further information - https://everse.software/RSQKit/greenphsecs_research_software_story

  https://github.com/UofM-Green-Compute/GreenPhysECS

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BACKUP Slides

Backup Slides

ECS Context

- Entity-Component-System (ECS) is a software development pattern that encourages the separation of data (components) from behaviour (systems)
- ECS programs are naturally concurrent, modular, and flexible

What is ECS

- Entities: The physical or logical object we are trying to simulate, **e.g. a particle**
- Components: Data associated with an entity, **e.g. the particle's velocity**
- Systems: Functions to alter the components of entities that match some criteria, **e.g. a collision system**

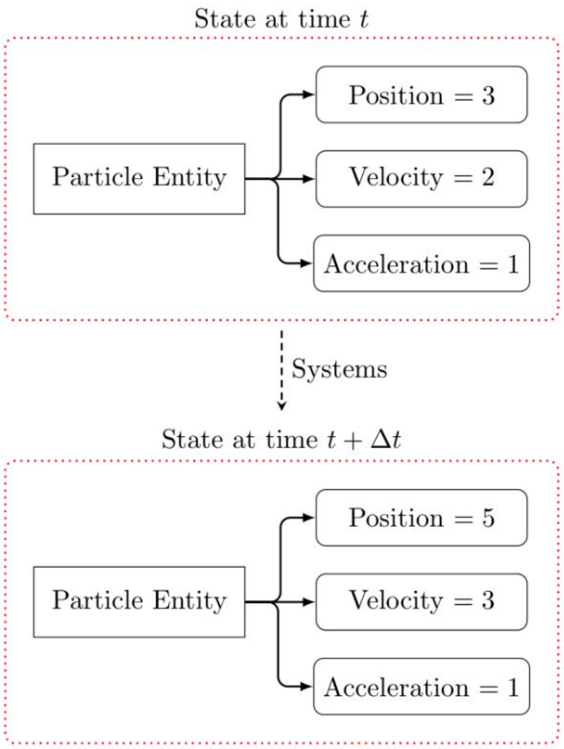

Figure 1: Diagram showing the evolution of the state of an ECS program. The state of the simulation is characterised by the entities and components. Systems evolve this state.

Modelling HUD Crop Epidemiology on a Lattice

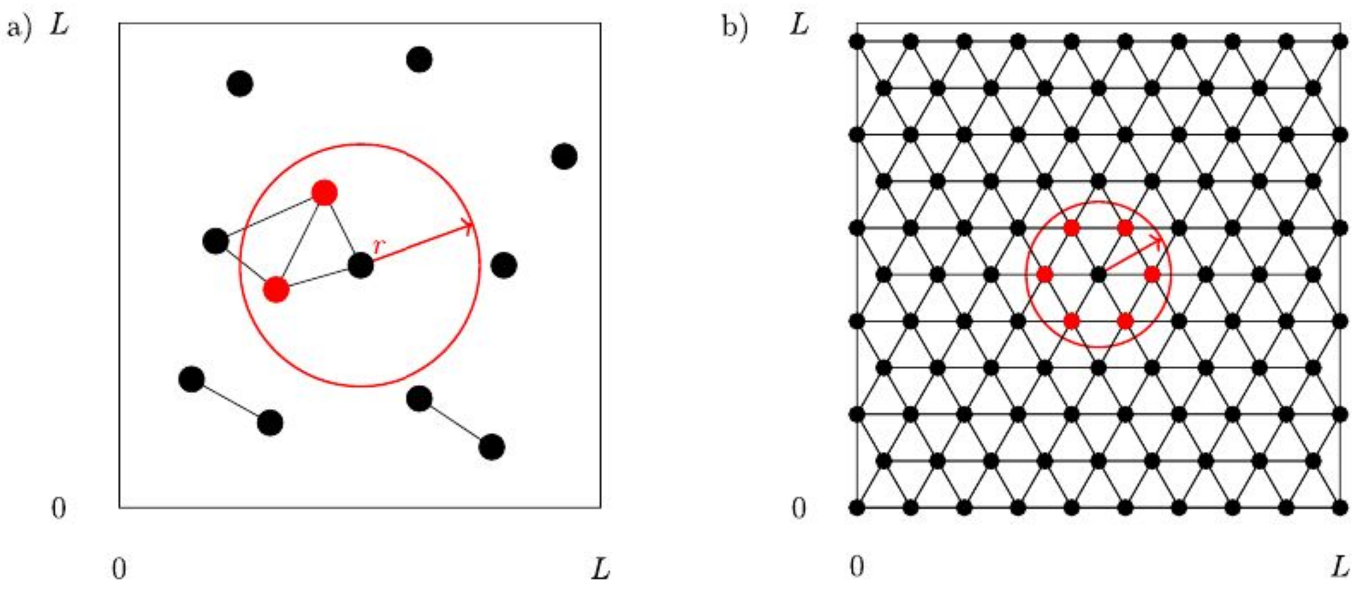

Figure 11: a) Plants are randomly placed in an $L \times L$ area. Plants within some radius, R, of each other are linked on a network. Linked plants can spread the infection to one another. b) Plants are placed in a hexagonal lattice in a $L \times L$ area. Similarly, all plants within R of each other are linked on a network.

Modelling HUD Crop Epidemiology on a Lattice

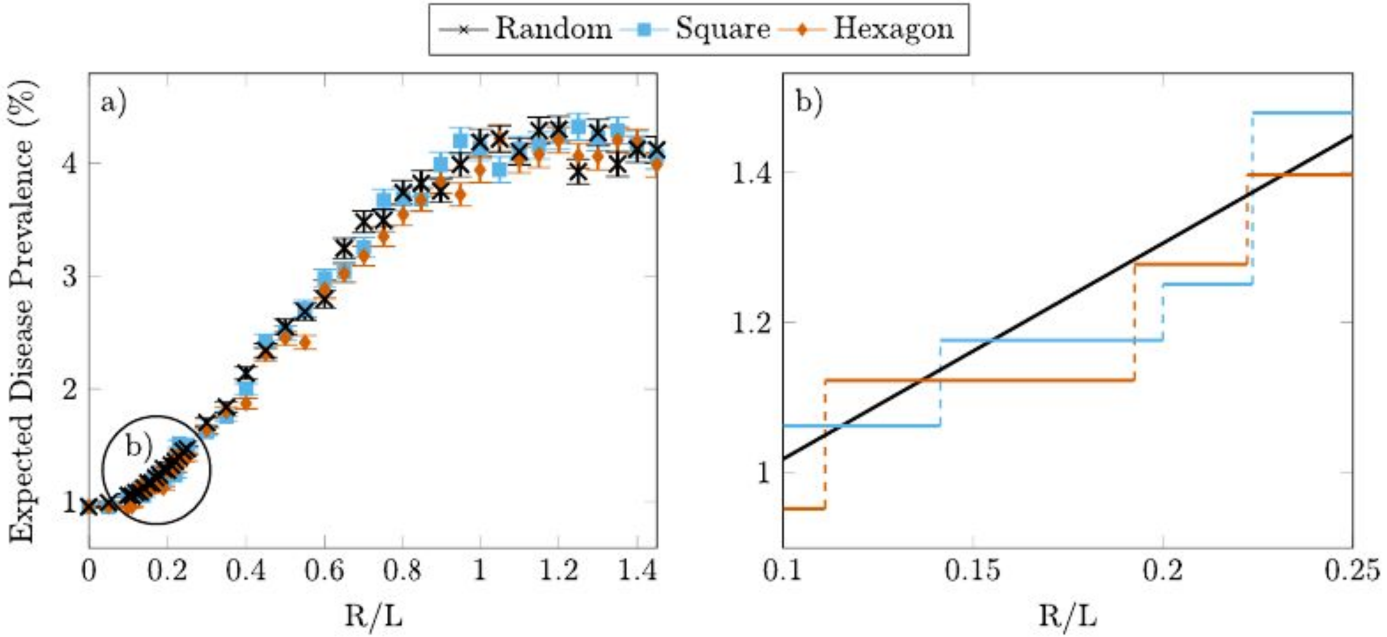

Figure 12: a) The *EDP* for infection radii between 0 and 1.45L, where L is the box length. b) A closer look at the *EDP* for infection radii between 0.1L and 0.25L with particular emphasis on the plateau behaviour of the lattice cases.

Early Detection of Disease Outbreak in Crops - HUD Model