How do spatial heterogeneity and dispersal in weed population models affect predictions of herbicide resistance evolution?

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ARTICLE INFO

Article history:
Received 21 March 2017
Received in revised form 4 July 2017
Accepted 3 August 2017

Keywords:
SOMER
Herbicide resistance
Evolution
spatial modeling
Simulation

ABSTRACT

Weed population simulations can be useful to predict the effects of alternative management practices on herbicide resistance (HR) evolution. Almost all previous simulations have ignored the possibility of within-field spatial structure in a weed population, instead making the implicit assumption of perfect dispersal and spatial homogeneity in population density and genetics. The effects of this simplifying assumption have not been examined, despite the fact that dispersal limitations and spatial structure within the population are likely to occur and to affect the evolution of resistance. Therefore, we developed a new spatially-explicit model called SOMER, and examined how changing the following factors affected the predicted evolution of resistance: the degree of spatial resolution used in the model; whether resistance was semi-dominant or fully-dominant; distances of pollen and natural seed dispersal; and inadvertent collection and grain harvester weed seed dispersal (GHWSD). Simulations showed that spatial resolution is important when modelling HR evolution, with the size of sub-population divisions, the pollen dispersal parameter, the level of dominance, and GHWSD all being important factors in predicting the rate and type of HR evolution. Our results show that accounting for spatial structure and dispersal does affect predictions of HR evolution, with the non-spatial model generally predicting faster resistance evolution compared to the more realistic equivalent spatial model. Most importantly, GHWSD increased the speed of HR evolution. Our spatial model also allowed us to investigate the dynamics of density and genetic structure within patches of herbicide resistant weeds, and we found that resistance genes were spread several times wider than the visible patch, and that homozygous mutations were commonly found in more centrally located weeds. We conclude that an ‘integrated spatial modelling’ approach that accounts for spatial structure should be considered when modelling HR evolution, and the evolution of resistance in general.

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1. Introduction

Herbicide resistance (HR) in agricultural weeds has evolved in many countries as a consequence of the widespread and persistent use of herbicides (Heap 2017). Adoption of no-till farming systems increased grower reliance on herbicides, resulting in an increase in herbicide resistance. One common farmer response to herbicide resistant weeds is to use alternative herbicides to regain weed control. However, increasing demands for alternative herbicides have not been matched by a satisfactory rate of new herbicide discovery and registration. In addition, once HR is established within weed populations, it may be difficult to remove. The paucity of usable herbicides to control weeds has led to a higher priority for responsible stewardship of herbicides, which is now being globally advocated (Norsworthy et al., 2012).

While several farming practices are commonly acknowledged as slowing the speed of resistance evolution (Norsworthy et al., 2012), new populations of herbicide resistant weeds are still appearing (Heap 2017). More work is needed to identify and quantify the role of specific practices in delaying the evolution of herbicide resistant populations. Typically, early in the evolution of a resistant population, there is a ‘latent’ stage where weed numbers are low whilst the frequency of resistance genes in the population is being enriched. This stage is largely invisible in the field, thus it is difficult to track early resistance evolution through field observations alone. However, once the resistant weeds are at high frequency in the population, herbicide failure can rapidly follow, illustrating the importance of the early latent stage. By allowing us to focus on and understand this stage, simulation modelling can aid in the early
identification of farming practices more likely to delay resistance evolution and keep weed numbers low.

Previous modelling of the evolution of HR had largely assumed, at least implicitly that there is spatial homogeneity of both weed seeds and resistance genes (reviewed in Renton et al., 2014; Bagavathiannan and Norsworthy 2016). For example, weeds in a field are often represented as a single population, with equal competition, and random mating (of cross-pollinating species) equally possible between all individuals across the field. In reality, weeds are often patchy in their distribution. Spatial distinction within a crop field means there can be local variations in resistance gene frequency or weed density, and growth reduction due to localised competition within weed patches. Localised variations in gene frequency can lead to localised genetic drift, which in turn can result in local gene extinctions, or concentrations of particular genes within cross-pollinated plants. In particular, allowing all weeds within any simulated large agricultural field to freely interbreed each year appears to be an unreasonable assumption (reviewed in Renton et al., 2014). Predictions and recommendations generated using models that account for spatial heterogeneity are thus likely to be more accurate. However, the effect of spatial heterogeneity in weed populations on resistance evolution has not been explored.

There are examples of spatially-explicit models of HR evolution, but these studies have generally not investigated whether the specific spatial location of individual plants makes a difference to modelled predictions. Previous spatial modelling of HR often focussed on how variation in the landscape can influence the spread of resistance evolution, but still represented populations within a field (or environment) as homogeneous (Roux and Rebound 2007; Richter 2008; Roux et al., 2008). Some spatial modelling of HR has recognised that weed populations within a field are not homogeneous, and examined the spread of specific genes (Richter et al., 2002; Richter and Seppelt 2004; Rummeland et al., 2012). However, no study has clearly investigated to what extent and in what ways spatial heterogeneity will affect simulated predictions of HR evolution.

Spatial structure within weed populations will influence resistance evolution due to the movement of genetic material within the simulated area. Pollen and seed are dispersed within the field both by natural effects and by human activities, with weed seed dispersal by harvest machinery possibly one of the most important factors in moving herbicide resistant weeds throughout a crop field (Barroso et al., 2006). Many of the weed species that are problematic in crops retain their seeds at maturity at a height that ensures collection by the grain harvester (Walsh and Powles, 2014). This ‘harvested’ weed seed is immediately fanned out behind the grain harvester and thus dispersed across the field (Blanco-Moreno et al., 2004).

Gene flow within a simulated area will also be affected by the specific characteristics of the resistance genes. Herbicide resistance can be conferred by genes encoding traits with varying levels of dominance, which will interact with spatial structure in the population. Spatial modelling allows us to account for natural and human-mediated gene flow and its interaction with different levels of dominance in predicting HR evolution, which is simply not possible with non-spatial models. In addition, none of the previous spatially-explicit field-scale modelling of HR (Richter et al., 2002; Richter and Seppelt 2004; Rummeland et al., 2012) has examined how the parameterisation of the pollen and natural seed dispersal functions will affect predictions of HR evolution at the field scale.

The first aim here is to: (1) develop a spatially-explicit weed model of HR evolution, and then use this model to test whether a spatially-explicit model gives different predictions to a non-spatially-explicit model; (2) test how the predictions of a spatially-explicit model were affected by semi-dominant vs fully-dominant resistance; (3) investigate alternative parameterisations of dispersal functions mimicking the natural spread of pollen and seeds; (4) investigate the effects of inadvertent grain harvester weed seed dispersal (GHWSD) during crop harvest.

2. Methods

2.1. Model structure

2.1.1. Model overview

To address the aims of this study, a new spatially-explicit individual-based stochastic model, the Spatially Orientated Model of Evolutionary Resistance (SOMER), has been developed to simulate the evolution of resistance in weeds infesting a crop field. Essentially, aspects related to spatial structure and the dispersal of pollen and seeds within a field have been added to our earlier non-spatial model (Somerville et al., 2017). In the new SOMER model, the simulated crop field area is evenly subdivided into square sectors, similar to a checkerboard, each with an associated sub-population of weeds. The term ‘integrated spatial modelling’ has been chosen to describe this type of model, where every plant and weed seed within the field area is accounted for, along with their individual age, location and resistance genetics. Squares have been chosen as the best sector shape as they align with activities such as crop seeding and harvest. The weed seeds are assumed to germinate and emerge throughout the growing season, modelled as discrete sequential weed cohorts (Fig. 1), in the same way as our previous non-spatial model. The earliest emerging weeds (prior to crop seeding) are classified as cohort one, with subsequent subdivisions between weed cohorts based on sequential annual activities such as herbicide application dates. The new model tracks the number of weeds of each genotype, in each cohort, in each sector of the simulated area, in each year, as well as the seeds of each genotype within the soil seedbank, within each sector.

Competition between weed cohorts and crop plants is modelled in the same way as in our non-spatial model (Somerville et al., 2017), using a hyperbolic competition function (Fixbank and Watkinson 1986; Somerville et al., 2017) to predict the number of weeds/m² and their subsequent seed production, except that competition is modelled separately within each sub-population (i.e. within each sector). Weed numbers are capped at a maximum density of 100 plants/m² via a non-selective cull, and model calibration was used to give realistic results (Somerville et al., 2017). Interactions between sub-populations by dispersed pollen and seed occur after determination of the amount of weed seed produced by each sub-population. To maintain consistent language it is written that ‘seed dispersal’ is the spread of weed seeds between sectors, whereas pollen travels within and between sub-populations, which are growing within sectors. Sector size is invariant within each simulation, whereas the size of each sub-population is dynamic, and influenced by annual processes such as herbicide application, competition, seed dispersal, and the evolution of resistance. The model is implemented in the ‘R’ language (R Core Team, 2014), and the model code is available on request from the authors.

2.1.2. Genetics

While our model can simulate the inheritance of up to six resistance genes using independent assortment, here we modelled resistance conferred by a single gene. The weed is assumed to be obligate cross-pollinating and diploid, with individuals possessing three possible genotypes: homozygous susceptible (SS), heterozygous resistant (RS) or homozygous resistant (RR). The genotype of each new seed is determined stochastically from a hereditary transition matrix (Richter et al., 2016). Mating is random, with restrictions imposed by cohort-based fitness and a sector-based pollen dispersal function. The cohort-based fitness weightings are based on the premise that plants emerging earlier will be bigger.
and likely to contribute more seed and pollen to the new seedbank. The weed numbers/m² in the results section incorporate this cohort-based fitness to translate results for all cohorts into a single ‘standard plant equivalent’ in the same way as our previous study, to allow better comparative analysis (Somerville et al., 2017). The sector-based pollen dispersal weightings are detailed below. Within each sub-population and weed cohort, the weeds are also classified into groups by their genotype. The initial frequency of heterozygous resistant seeds is a model parameter, as is the mutation rate (the probability of the formation or loss of new mutations via meiotic change). New random genetic mutations are simulated within each season’s new seeds, using probability transition matrices (Somerville et al., 2017).

2.1.3. Dispersal of pollen and seed

2.1.3.1. Pollen dispersal function. To achieve the aim of having a fully integrated spatial model, it is necessary to include every plant within the designated area as a potential pollen source. A Weibull function has previously been fitted to data from Knowles and Ghosh (1968) to calculate the probability that a seed is pollinated by each plant in the simulated area (Somerville and Renton 2015).

\[
pollination\, probability_i = \frac{e^{-a \left( \frac{\text{distance}_{ij}}{2017} \right)}}{\sum_{j=1}^{n} e^{-a \left( \frac{\text{distance}_{ij}}{2017} \right)}}
\]

The current parameterisation of this function included further minor refinement to account for edge effects and self-pollination in their 1968 data. The Weibull function was chosen over the exponential and Cauchy functions as it gave a better fit by non-linear least squares regression (Fig. A1A). In this Weibull function, \(a\) is the slope parameter, \(n\) is the total number of flowering plants in the simulated area, and ‘distance’ is defined as the distance between the centre of the sector containing the mother plant and the centre of the sector containing the \(i^{th}\) pollen donor plant (measured using Pythagoras’s Theorem). When the mother plant and the pollen donor plant are growing within the same sector \(\text{distance} = \frac{1}{2} \sqrt{\text{sector area}}\). The denominator in this function ensures that the probabilities across all potential pollinating plants sum to one. The slope parameter \(a\) defines the rate that probability decays or declines with distance, and can be varied to represent different pollen dispersal characteristics. These refinements yielded a slope parameter \(a = 6.424\). This value is hereafter called the high slope parameter. However, this parameterisation does not fully account for the influence of intervening crop and weed plants that can limit pollen dispersal (Murray et al., 2002), meaning that shorter distances for pollen dispersal are more likely. Therefore, an alternative parameterisation of the pollen dispersal function was calculated using halved distances; best-fit estimations yielded the same shape factor \((0.2498)\) and scale parameter \((0.9136)\) with a different slope parameter \(a = 7.637\). This value is hereafter called the medium slope parameter. A smaller slope parameter has also been generated, using an evenly spaced log transformation, such that the low slope parameter \(a = 9.079\). Further details of the calculation of this low slope parameter, and the effect on pollen dispersal of these alternate slope parameters, are provided in Appendix A (Fig. A1B).

As an alternative to ‘full pollen sharing’ across the entire simulated area, ‘limited pollen sharing’ can be implemented for individual sector interactions with pollination probabilities that fall below \(10^{-3}\). With ‘limited pollen sharing’, pollination probabilities less than \(10^{-8}\) are rounded to zero, which expedites the running of the simulations. In preliminary simulations, this limit on the pollen dispersal distance did not noticeably affect the results (data not shown).

2.1.3.2. Natural seed dispersal function. Natural seed dispersal is defined here as the probability of seed moving away from its maternal sector to adjacent sectors. In reality, this would be influenced by biological and environmental factors such as seed height, plant density, weather, insects, and farming activities (inadvertent weed seed collection and dispersal by a grain harvester is represented with a separate function) (Bergelson et al., 1993; Chambers and MacMahon 1994; González-Andújar and Saavedra 2003; Cousins et al., 2008). Seed that disperses naturally outside its maternal sector is assumed to spread primarily into the four directly adjacent sectors, with a small amount moved further laterally, into the four diagonally adjacent sectors. This natural seed dispersal represents all seed movement occurring between weed seed shed in spring until weed germination. It is assumed that dormant seed in
the soil does not move any further after its first autumn because there is minimal soil movement with conservation tillage machinery (Cardina et al., 1996; Aguiar and Sala 1997). Probability of seed dispersal over the edge of the maternal sector (into the four directly adjacent sectors) and into the corner sectors is dependent on two parameters, the proportion of seed loss per square metre (w) and the sector area (b). Specifically, the probability of weed seed moving out, into each directly adjacent sector (s), or into each corner adjacent sector (c), is governed by the following functions

\[ s = w(510^{0.5-2})/200b \]

The corner sector dispersal (c) is assumed to be two percent of the total seed-dispersal from a 1 m² sector. The relatively small size of c is due to limitations on diagonal seed movement imposed by crop plants and stubble. The probability of seed dispersal is assumed to be the same for all seeds produced inside each sector (independent of genotype or maternal cohort). The functions for calculating the natural seed distribution at different sector sizes (Eq. (2)) ensure that the same amount of seed will be spread sideways per metre of sector boundary, and the same amount will be spread into the diagonal corners, thereby maintaining consistency independent of sector size. The mathematical demonstration of this consistency is provided in Appendix B.

2.1.3.3. Grain harvester weed seed dispersal (GHWSD). Weed seeds that are intact and still attached to their plant at the time of grain harvest are inadvertently collected into the grain harvester, then evenly dispersed across the width (12 m) of the harvester, and longitudinally dispersed for up to 60 m, along the harvester path. The harvester tracks a back-and-forth pattern across the field area and is assumed to closely follow GPS guidance (Tullberg et al., 2007), so that during sequential annual harvests the harvester always follows exactly the same path (see also Section 2.1.3.4 ‘Edge effects’, below). The longitudinal distance of GHWSD used in this study is set at 5 m backward and 55 m forward, along the direction of harvester movement. Collected weed seed is dispersed over this 60 m distance using 10 different probabilities of the seeds being dropped, from back to front along the 60 m, with the values of 0.02, 0.22, 0.26, 0.23, 0.1, 0.07, 0.05, 0.03, 0.01 and 0.00. These numbers are based on measurements of annual ryegrass seed dispersal during harvest of a wheat crop in Spain (Blanco-Moreno et al., 2004), with the distances increased here due to the comparatively faster harvester ground speeds common in Australia. Further explanations and dispersal probability graphs illustrating the extent of seed movement during harvest are included in Appendix C. Some weed seeds within the field are not collected by the grain harvester because the weed seeds are below the cutter bar, or have already been shed, prior to harvest. The fate of both uncollected seed, and previously harvester-dispersed seed, then follows the natural seed dispersal functions defined in Section 1.3.2. The probability of a seed produced in a given season being collected into the front of the harvester is 1–seeddrop, where seeddrop is a model parameter representing the proportion of seed that drops pre-harvest or is not collected for any other reason (Walsh and Powles 2014). If the annual maximum harvester seed dispersal distance is 55 linear metres, then in 5 years resistance could spread 275 linear metres via harvester seed dispersal alone. Simulations involving GHWSD are therefore confined to field areas of at least 10 ha. Additionally, the harvester width of 12 m limits simulations including GHWSD to sector sizes of 144 m² or less.

2.1.3.4. Edge effects. Designing spatial models requires decisions to be made concerning seed and pollen dispersal from plants growing close to the edge of the simulated field area. We generally used ‘wrapping’, where the left and top edges of the simulated area are assumed to wrap around and meet the right and bottom edges, respectively. This is equivalent to assuming the simulated area is one of a number of identical areas adjoining on all sides and diagonals. A different, ‘not wrapped’ approach was used in simulations investigating the radial spread of resistance from a single centrally placed resistant seed, where we can assume that the simulated area is surrounded by a larger field area containing no resistant weeds. This larger area was incorporated into pollen flow calculations with the assumption that plants in the surrounding un-simulated areas had similar density and susceptibility levels to the plants on the edges of the simulated area. A maximum density of 7 ‘standard plant equivalent’ weeds/m² was imposed on each sector to stop random outbreaks of resistance in the plants on the edges of the simulated area having an undue influence on the results. A maximum density of 7 weeds/m² was chosen as it is greater than occurred in simulations run without resistance genes (results not shown).

2.1.4. Computer speed, field area and sector sizes

In this study, computing speed is governed by the number of genes, cohorts, and sectors, rather than the number of individual plants, because weeds are grouped by their genotype and cohort within each sub-population. Two sub-functions, for ‘full pollen sharing’ and the ‘formation of new genetic mutations’, are the most taxing for computing speed. To increase speed, the ‘full pollen sharing’ can be replaced with ‘limited pollen sharing’ and the ‘formation of new genetic mutations’ can be turned off, without having a large influence on the results (data not shown). The only exception was that the formation of new genetic mutations was important in simulations that ran for a long time, and where the weed control strategies were effective enough to eliminate the initial resistance genes from the field (results not shown).

Faster computer simulations of large field areas can be implemented by using fewer (larger) sub-populations. Some advantages of larger field areas are that they allow rarer resistance alleles, gene interactions, and lower new resistance gene mutation frequencies to be simulated more consistently. However, finer spatial distinctions are lost when using larger sectors. An upper limit of around 10,000 sub-populations currently exists on the available computer (with an Intel® core™ i7-4770CPU® 3.40 GHz processor, 28 GB of RAM and a 64 bit O.S.), whilst running SOMER (when run with two genes), with the sub-functions for ‘limited pollen sharing’ and the ‘formation of new genetic mutations’ both turned on. This is the sub-function configuration used in the following simulation studies.

2.2. Simulation studies

Four studies were designed to address each of the four aims of this investigation, with each study including a number of contrasting scenarios (Table 1). Ten replicate simulations of each scenario were run, to account for stochastic variability. A difference between scenarios equal to or greater than one year of effective herbicide use was designated as a criterion for ‘effective difference’.

2.2.1. Parameterisation

The standard scenario of herbicide applications is described in Fig. 1, with the parameters listed in Table 2. For simulated areas above one hectare, which initially contained more than one heterozygous resistant seed, we used ‘wrapping’ to account for edge effects, and the ‘not-wrapped’ approach was used for the one hectare field area when it was used in studies 2 and 3, as they initially contained only one centrally placed heterozygous resistant seed (see Section 2.1.3.4).

The scenarios were parameterised to simulate the evolution of single gene resistance to a post-emergence herbicide in obligate cross-pollinated annual ryegrass (Lolium rigidum) within a wheat
Table 1
Parameter values examined in these computer simulations.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Study one</th>
<th>Study two</th>
<th>Study three</th>
<th>Study four</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Probability that any seed in the initial population will be heterozygous resistant.</td>
<td>$1 \times 10^{-5}$</td>
<td>1 in 1.17 ha $(1.45 \times 10^{-6})$</td>
<td>1 in 1.17 ha $(1.45 \times 10^{-6})$ &amp; $1 \times 10^{-6}$</td>
<td>$1 \times 10^{-5}$ &amp; $1 \times 10^{-6}$</td>
<td>Higher resistance levels were needed in smaller field areas.</td>
</tr>
<tr>
<td>Simulated field areas</td>
<td>10.5 ha</td>
<td>1 ha</td>
<td>1 ha &amp; 10.5 ha</td>
<td>10.5 ha &amp; 42 ha</td>
<td>Smaller fields contain smaller populations, and the absolute number of initially resistant seeds affected variability.</td>
</tr>
<tr>
<td>Sector sizes</td>
<td>9m², 36m², 144m², 1296m², 6561m², 26244m² and non-spatial</td>
<td>1m² &amp; 9m²</td>
<td>1m² &amp; 144m²</td>
<td>9m², 36m², 144m²</td>
<td>Computer constraints limited the maximum number of sub-populations to around 10,000. This meant that smaller field areas needed to be used in simulations with finer spatial resolution.</td>
</tr>
<tr>
<td>Dominance</td>
<td>Semi-dominant resistance (70% survival of heterozygote)</td>
<td>Semi-dominant resistance (70% survival of heterozygote) &amp; Fully-dominant resistance</td>
<td>Semi-dominant resistance (70% survival of heterozygote)</td>
<td>Semi-dominant resistance (70% survival of heterozygote)</td>
<td>Semi-dominant resistance has seldom been simulated, but is commonly found in the field (Powles and Yu, 2010)</td>
</tr>
<tr>
<td>The slope parameter ($a$) influencing pollen dispersal distance.</td>
<td>Medium $a = 7.637$</td>
<td>Medium $a = 7.637$</td>
<td>High $a = 6.424$ Medium $a = 7.637$ Low $a = 9.079$</td>
<td>Medium $a = 7.637$</td>
<td>The true values for pollen dispersal within a wheat field are unknown. Pollen dispersal when constrained by inter- and intra-specific competition was explored.</td>
</tr>
<tr>
<td>The seed dispersal parameter ($w$), natural seed movement away from the maternal sub-population.</td>
<td>Medium $w = 4%$</td>
<td>Medium $w = 4%$</td>
<td>High $w = 20%$ Medium $w = 4%$ Null $w = 0%$ (no seed dispersed)</td>
<td>Medium $w = 4%$</td>
<td>The true values for ryegrass movement within a minimum till wheat crop are unknown.</td>
</tr>
<tr>
<td>Seed drop, the probability that seeds were uncollected by the harvester.</td>
<td>Seeddrop = 1, seeds were not collected by the grain harvester</td>
<td>Seeddrop = 1, seeds were not collected by the grain harvester</td>
<td>Seeddrop = 1, seeds were not collected by the grain harvester</td>
<td>Seeddrop = 1, &amp; Seeddrop = 0.12, most weed seeds entered the harvester each year.</td>
<td>The effects of inadvertent weed seed collection and dispersal by a harvester (GHWSD) on resistance evolution are unknown</td>
</tr>
</tbody>
</table>
crop growing in a southern Australian Mediterranean-type climate. Populations of annual ryegrass now found in many southern Australian cropping fields typically exhibit high levels of resistance to at least one post-emergence herbicide (Llewellyn et al. 2009; Boutsalis et al., 2012; Owen et al., 2014). Parameter values (Table 2) were within the range used in our previous non-spatial model (Somerville et al., 2017), which were in turn based on similar models such as RIM (Pannell et al., 2004; Lacoste and Powles, 2014) and PERTH (Renton et al., 2011).

2.2.2. Study details

2.2.2.1. Study one. The first study addressed aim 1, to discover whether a spatially-explicit model of HR evolution gives different predictions to a non-spatially-explicit model. Study one examined the effects of alternate spatial resolution on the growth of the evolving resistant population, and how this affected the average weed density and the levels of homozygous resistance (Table 3). A 10.5 ha area, with different spatial resolutions and an initial resistance gene frequency of 1 x 10^-5, was used for the simulations in this study.

2.2.2.2. Study two. Study two addressed aim 2, to investigate the influence of semi-dominant vs fully-dominant resistance on the number and spread of resistant weeds. Study two started with a single heterozygous resistant seed in the centre of a one hectare area in the first year, and used a finer spatial resolution of 1 m^2 and 9 m^2 sectors.

2.2.2.3. Study three. Study three addressed aim 3, to determine how alternative parameterisations of pollen and natural seed dispersal affected predictions of the evolution of herbicide resistance. Study three examined how three alternative parameterisations of pollen dispersal (a) and natural seed dispersal (Sm) affected the growth and spread of an herbicide resistant weed population (Table 4). The effects of these alternate parameterisations were considered for two cases. The first utilised a larger sector size and field area; the results of study one indicated that sectors of 144 m^2 were stable in SOMER, and generated low levels of variability between replicates. The use of 144 m^2 sectors enabled a larger field area, of 42 ha to be simulated. This larger field area permitted a more realistic, lower, initial resistance gene frequency of 1 x 10^-6. The second case examined resistance spread from a single centrally positioned resistant weed at a finer resolution, utilising 1 m^2 sector divisions within one hectare area.

2.2.2.4. Study four. The fourth study addressed aim 4, the effects of grain harvester weed seed dispersal (GHWSD) on the evolution of herbicide resistance. Three simulations were repeated from study one, (a 10.5 ha area, with spatial resolution of 9 m^2, 36 m^2 and 144 m^2, identical number and placement of seeds at the start of the second growing season (Section 2.3), and the probability of heterozygous resistance in the initial population of 10^-5), with the addition of seed dispersal by the harvester (Table 1). Study four also included simulations of a larger field area of 42 ha, thereby allowing a heterozygous resistance frequency of 10^-6 to be used; and an examination of alternate sector sizes of 36 m^2 and 144 m^2, with, and without, harvester seed dispersal.

2.3. Preliminary investigations and alternative simulations

Preliminary studies were conducted to identify appropriate sub-population and field sizes and an initial resistance gene frequency that together gave reasonably precise replicates. We found that in many cases where field areas were small, none of the resistant seeds survived to establish resistant populations. In other cases, with initially low numbers of resistant seeds, stochastic variation between simulated replicates obscured differences between the scenarios. We identified that the major source of stochastic variation was the number and location of resistant plants surviving the first year. On average, for every 100 fully-dominant resistant seeds at the start of the first year, there were 8 ‘standard plant equivalent’ (Somerville...
et al., 2017) weeds surviving to reproduce at the end of the first year. This reduction, from 100 seeds down to 8 ‘standard plant equivalent’ individuals at the end of the first year, was caused by several factors, including: the pre-seeding knockdown herbicide mortality, the reduced size of weeds in later germinating cohorts, the stochastic nature of germination and seed survival, and the low frequency of the initial resistant seeds. Consequently, there was high variability in the number of resistant plants surviving the first year, as well as high variability in their location within the simulated area. In contrast, these processes in later years caused little additional stochasticity, as resistant weeds surviving and reproducing at the end of the first growing season had an almost 100% probability of going on to create patches of resistant weeds in subsequent years. To reduce the stochastic variation between replicates due to these first-year effects, we also conducted alternate spatial simulations with an identical number and placement of seeds at the start of the second growing season. These alternate spatial simulations were confined to comparisons between different scenarios conducted on the same field area. Their reduced variability generated a clearer view of the comparisons relating to our aims, whilst simulations with full variability generated a better understanding of the biological importance and consistency of these comparisons.

3. Results

3.1. Study one: spatial and non-spatial models and alternate spatial resolution

When the SOMER model was used without spatial divisions, and with an initial single semi-dominant resistance gene frequency of $1 \times 10^{-3}$, resistance to a post-emergence herbicide evolved rapidly, around year six (Fig. 2A). However, when spatial divisions were included (creating spatial heterogeneity using somewhat independent sub-populations of the weed, each within its own square sector), resistance evolved more slowly, around year 7 (Fig. 2A). Varied spatial resolution, which created sectors from $9 \text{m}^2$ up to $324 \text{m}^2$, all gave surprisingly similar results, and slowed resistance evolution, in comparison to the non-spatial simulations (Fig. 2A). In addition, these smaller sector sizes increased the level of homozygous resistance to higher than that simulated without spatial divisions (Fig. 2B). This is logical, due to cross-pollination occurring more frequently between closely neighbouring plants. Within SOMER, closely neighbouring weeds either are within the same sub-population, or are within adjacent sub-populations, in bordering sectors. As expected, when sectors were larger, the spatial model simulated identically to the non-spatial model (Fig. 2C&D). At sector sizes greater than $6561 \text{m}^2$ there were no differences between simulations conducted using the spatial and non-spatial models. The sector size of $1296 \text{m}^2$ gave intermediate results, with large variability between replications (Fig. 2C&D). Almost all the sub-populations within sectors larger than $1296 \text{m}^2$ contained more than one resistant seed at the start of the simulations (Table 5) meaning that they did not suffer the early check in resistant weed growth (caused by genetic drift and local extinctions) that occurred in simulations utilising smaller sectors (Fig. 3).

3.2. Study two: fully dominant resistance with finer spatial resolution

Herbicide resistance, when conferred by a single gene, is usually semi-dominant (Darmency 1994); consequently, semi-dominant resistance has been chosen as the default in these studies. When semi-dominant single gene resistance evolution of a single patch of resistant weeds was modelled with a fine spatial resolution ($1 \text{m}^2$ and $9 \text{m}^2$), a large growth in weed numbers only occurred in the small central part of a much larger area of the field that contained resistant seeds. This resistance produced an obvious localised change in weed density at the start of the 5th season (Fig. 4); however, any earlier than this the patches would likely be too small and not dense enough for a farmer to identify in the field (data not shown). This central area corresponds to the part of the field containing many homozygous resistant weeds (Supplementary Fig. S2). When semi-dominance is assumed in the SOMER model, 95% of the homozygous individuals, but only 70% of the heterozygous plants, survive herbicide application, and thus the former will produce more seed. In contrast, where simulations assume full dominance of the resistant gene, 95% of both the homozygous and heterozygous individuals survive herbicide application. Consequently, when fully-dominant single gene resistance evolution of a single patch of resistant weeds was modelled, this led to the growth of a dense weedy patch that extended further across the field than for semi-dominant resistance (Fig. 4, upper tier: compare A vs. B and C vs. D), but still not as far as the extent of the resistant seeds (Fig. 4, lower tier). The patch extended across areas of the field containing both homozygous and heterozygous resistant individuals (Supplementary Fig. S2). Overall, assuming a fully-dominant resistance gene within the simulations increased

<table>
<thead>
<tr>
<th>Pollen dispersal function slope parameter ($\alpha$)</th>
<th>Natural seed dispersal parameter ($\omega$)</th>
<th>Probability that pollen is sourced from a plant within its own sub-population</th>
<th>Probability that a naturally shed seed remains within its own sector</th>
</tr>
</thead>
<tbody>
<tr>
<td>'high' ($\alpha = 6.424$)</td>
<td>'high' ($\omega = 20%$)</td>
<td>0.816</td>
<td>0.983</td>
</tr>
<tr>
<td>'medium' ($\alpha = 7.637$)</td>
<td>'medium' ($\omega = 4%$)</td>
<td>0.920</td>
<td>0.997</td>
</tr>
<tr>
<td>'low' ($\alpha = 9.079$)</td>
<td>'null' ($\omega = 0%$)</td>
<td>0.974</td>
<td>1.000</td>
</tr>
</tbody>
</table>

Table 4 Specifications of alternate pollen and natural seed dispersal parameters, with a sector size of 144 m² and 1 m², used in study three.
Fig. 2. Changes in average weed density (A&C) and homozygous resistant weed percentages (B&D) resulting from simulations with different sector sizes within a 10.5 ha area, compared to a non-spatial model. Spatial simulations were compared to the non-spatial simulations, and conducted using both smaller sectors (A&B) and larger sectors (C&D). Plots show the means of 10 replicates, and include vertical bars showing ±1 standard deviation.

Table 5
Effect of sector size, with a field size of 10.5 ha, and an initial resistance probability of $10^{-5}$. Sub-population statistics in the early years (ten replicates, with standard deviations).

<table>
<thead>
<tr>
<th>Sub-population sector size (m²)</th>
<th>Initial population in the first year, proportion of sub-populations with:</th>
<th>Proportion of second year sub-populations with:</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>No resistance</td>
<td>One resistant seed</td>
</tr>
<tr>
<td>9</td>
<td>0.989 ± 0.02</td>
<td>0.011 ± 0.001</td>
</tr>
<tr>
<td>36</td>
<td>0.956 ± 0.003</td>
<td>0.043 ± 0.003</td>
</tr>
<tr>
<td>144</td>
<td>0.84 ± 0.02</td>
<td>0.15 ± 0.01</td>
</tr>
<tr>
<td>324</td>
<td>0.68 ± 0.02</td>
<td>0.26 ± 0.02</td>
</tr>
<tr>
<td>1296</td>
<td>0.19 ± 0.05</td>
<td>0.31 ± 0.03</td>
</tr>
<tr>
<td>6561</td>
<td>0.01 ± 0.03</td>
<td>0.01 ± 0.02</td>
</tr>
<tr>
<td>26244</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

the number of weeds, and also increased the percentage of heterozygous individuals (Supplementary Fig. S3).

By the fifth year, resistant seeds could be found at the furthest edges of the one hectare area (Fig. 4, lower tier). There were empty sectors (areas of field without any weeds) within the 1 m² simulations (Fig. 4, lower tier, A&B), which occurred because post-emergence herbicide use resulted in the local extinction of several of the smaller sub-populations growing within the 1 m² sectors. In
contrast, none of the sub-populations within the larger 9 m² sectors were extinct (Fig. 4C&D). Despite these empty sectors in the 1 m² simulations, the resistant seeds (Fig. 4, lower tier) extended at least five times as far out into the field than the size of the dense patch of weeds (Fig. 4, upper tier) would suggest. This was true for both the dominant and semi-dominant resistance genes, and for the 1 m² and 9 m² sectors.

The finest spatial resolution of 1 m² (only possible within the smaller one hectare simulations), allowed a close examination of how resistant patches spread outwards, from one initial heterozygous resistant seed. As well as more extinct sub-populations, the simulations utilising 1 m² sectors were also more prone to losing all their resistance genes, via genetic drift. During the first year, in 46%–67% of the replicates, the sub-populations lost their resistant genes via genetic drift, with lower rates of genetic drift in the simulations with fully-dominant genes and also in the simulations with larger 9 m² sectors. Because of the large variability between replicates, simulations with identical seed distribution at the beginning of the second year were used in Fig. 4 and in Supplementary Fig. S3 (section 2.3).

3.3. Study three: varying pollen and natural seed dispersal

Dispersal of pollen and weed seed within a spatially modelled crop field is one of the defining characteristics of a spatial model, and a sensitivity analysis of the chosen dispersal functions gave some insight into the importance of this previously unexplored aspect of HR modelling. Changes to the pollen dispersal distance had a comparatively large effect on the simulated growth in weed numbers. When the average distance of pollen dispersal was increased, average weed density increased more rapidly (Fig. 5A). In contrast, similar changes in the natural seed dispersal rates made very little difference to the average weed density (Fig. 5B).

The level of variation between replicates changed at different pollen and seed dispersal parameters. In the 144 m² sectors, the
variability between replicates was greatest at the high pollen dispersal rate (Fig. 5A). In contrast, the variability between replicates in the 1 m² sector divisions was greatest at the medium pollen dispersal rate (Supplementary Fig. S4A).

The localised sub-population extinctions that occurred within the 1 m² sectors (see Section 3.2) meant that alterations to the pollen and seed dispersal parameters were more important when using 1 m² sectors (Supplementary Fig. S3, S4&S5). Increasing the pollen dispersal distance had a large effect on the growth in weed numbers and on the spread of resistance genes between the 1 m² sectors (Supplementary Fig. S6 A&B&C). Changes in the natural seed dispersal parameter had less effect on both weed numbers and heterozygosity, but had a large effect on the number of empty 1 m² sectors (Supplementary Fig. S6 D&B&E). Movement of seed across the field was needed to repopulate empty sectors.

In Study two (using 1 m² and 9 m² sectors), areas of the field experiencing a rapid growth in weed numbers also developed a high level of homozygosity, particularly within simulations of a semi-dominant resistance genes (see above). This relationship still existed in Study 3 (utilising 144 m² sectors), but was less evident and was further lessened in simulations with a ‘high’ pollen dispersal rate (Supplementary Fig. S5). The pollen spread function is designed to disperse the same amount of pollen the same distance, despite alternate simulations utilising different sector sizes, but because the centres of larger sectors are further apart, there is a higher probability that resistant pollen is retained within large sectors (Table 4).

3.4. Study four: grain harvester weed seed dispersal (ghwsd)

Mature weed seeds that are retained on the mother plant are routinely ‘harvested’ alongside the crop. Typically, this harvested weed seed is uniformly spread from the rear of the grain harvester as it traverses the crop field. Harvesters are designed to spread crop residues, protecting the soil from erosion and water depletion, and facilitating no-till seeding. In these simulations, GHWSD was found to increase the growth in weed numbers, so that HR evolution occurred one year earlier compared to the same spatial simulation without GHWSD (Fig. 6A). In addition, GHWSD increased the percentage of heterozygous individuals (Fig. 6B). Each year, GHWSD spread the resistant weeds further across the field (Fig. 7), and the weed infestation showed a clear stripe pattern due to linear dispersal by the grain harvester. Weed densities within the harvester ‘tails’, deposited behind the GPS guided harvester, were lower than the density within the un-spread patches, (Fig. 7), and this decrease in density lowered intra-specific competition. Seed dispersal by the harvester also influenced the distribution of all seeds, with just one year of GHWSD creating a noticeably more evenly distributed weed seedbank (Supplementary Fig. S7).

When the simulations included GHWSD, selection of an appropriate sector size was less important. Changes in sector size had much less effect on weed numbers, homozygosity and the visual model outputs, when GHWSD was included in the simulations (Figs. 6 and 7). This is because, within SOMER, the same average GHWSD distances were maintained in different simulations, notwithstanding alterations in sector size (Appendix C, Fig. C1).

4. Discussion

Our first aim in this study was to test whether a spatially explicit model of herbicide resistance (HR) evolution gave different predictions to a non-spatially-explicit model. Using the newly developed SOMER model, we found that HR evolution was predicted to occur more slowly when a spatial structure (allowing spatial heterogeneity) was included in a HR model, compared to a non-spatial model (Fig. 2). In a non-spatial model, resistant plant populations within
Fig. 6. Effects of seed dispersal by the grain harvester and sector size (36 m² or 144 m²) on the average weed density (A) and homozygous resistance levels (B) simulated over a 42 ha area. The probability of heterozygous resistance in the initial seed population is $10^{-6}$. Plots show the means of 10 replicates, and include vertical bars showing ±1 standard deviation.

Fig. 7. Illustration of how spatial patterns in weed density are influenced by seed dispersal by a grain harvester (top row), or without seed dispersal by a harvester (bottom row) across alternate sector sizes. These seven panels show a 10.5 ha area. All simulations had identical seed distribution at the beginning of the second year (Section 2.3), and show weed numbers/m² seven years after herbicide use began. The figures were chosen as representative of the seven scenarios (each one was selected from ten replicates). The white arrows point out new outbreaks of resistance, unique to each simulation.

A simulated field can increase rapidly, since the plants only become density-constrained when the whole population is very large. Until then, the surviving resistant individuals are assumed to grow normally, unchecked by intra-specific competition, and to freely share their resistant pollen and seeds across the whole field and population. Conversely, in a spatial model, resistance genes initially
establish in only a small proportion of possible locations and then have to spread physically across the field, at a speed that is limited by seed and pollen dispersal rates. The resistant individuals surviving in the field are thus located within resistant patches, and are therefore in intense competition with close neighbours, which limits their growth. In all of those aspects where the spatial model differs from the non-spatial model, the spatial model would appear to be more realistic.

In addition to the slower growth in weed numbers, integrated spatial modelling predicted a higher percentage of homozygous individuals than a non-spatial model (Fig. 2). In these simulations, homozygosity required matings between two resistant individuals because the weed is an obligate cross-pollinating species. Therefore, when pollen dispersal is limited, a homozygous resistant seed is only likely to be created when two individual resistant plants grow close to each other. In the spatial model, and especially with smaller sectors, (less than 324 m²), plants have a propensity to breed with close neighbours who are more likely to be resistant, and also to drop seed close to themselves, thus creating more resistant individuals in close proximity in future generations. Therefore, from the third year onwards, homozygosity increased in the spatial simulations, with higher levels of homozygosity occurring in simulations with sectors less than 324 m² (Fig. 2).

The fact that the spatial model predicted a slower growth in weed numbers, and a higher proportion of homozygosity than was predicted in non-spatial modelling, has important implications. In previous studies, simulation results and comparisons between strategies have often been expressed in terms of the ‘year of failure’. For example, a seedbank with 20% of its individuals showing resistance (heterozygous or homozygous) has been taken to mean a failure of the weed management program (Neve et al. 2003). Alternatively, failure has been defined as the first year that weed numbers exceed a certain threshold (Renton et al. 2011). However, the results from this study imply that simulations expressing year-of-failure give different results when the simulations are altered to include spatial resolution. Moreover, these differences between simulations may become more- or less-favourable, depending on the assessment criteria, when studies include spatial structure. These conclusions indicate that the correlation between an increasing level of resistance and a sharp increase in weed numbers are more complex and subtle than is generally recognised, particularly when both vary highly across space as well as time.

There was a specific range of sector measurements, of between 9 m² and 324 m², which generated very similar results, and this similarity is assumed specific to the parameter values used in this study. The specific parameter values important here would be the density of the initial population, the initial concentration of resistance alleles, and the probability of death from herbicide application/s. In contrast, 1 m² sectors behaved differently here, probably because the finer spatial divisions generated empty sectors (with these parameter values). This was due to localised weed seed extinctions, where smaller populations are more likely to go extinct due to the effects of demographic stochasticity. Localised extinctions did not occur with sector sizes of 9 m² and larger. In addition, the loss of the resistance genes from sub-populations due to genetic drift occurred more frequently when smaller sectors were used, due to the higher proportion of smaller sub-populations that initially contained only one resistant individual (Table 5). Within the range considered in this study, the finer the scale of the model, the more realistic its representation of the real situation, and thus the predictions of the finer-scale model (slower evolution of herbicide resistance, higher levels of homozygosity, local extinctions of genes and populations, and resulting spatial structure) are likely to occur in reality as well.

Finer resolution (smaller sectors) has the added advantage of allowing better analysis and understanding of patch dynam-
landscape scale has previously been identified as important in the spread of resistance genes into uncontaminated fields (Déhy et al., 2010; Busi et al., 2011). Therefore, correctly determining the functional form and parameter values of the pollen dispersal function is an important factor in the spatial simulation of resistance evolution in a cross-pollinating species.

Grain harvester weed seed dispersal (GHWSd) was identified as an important factor in the field-wide spread and growth in numbers of resistant individuals, and was found to shorten the effective life of the herbicide by one year (Fig. 7). When implemented, GHWSd was the main factor affecting the spread of resistance across the field; similar findings were reported from early spatial modelling work by Maxwell (1992). In addition, harvesters disperse individual seeds more evenly (Supplementary Fig. S7), (Walsh et al., 2013; Martin et al., 2015), thereby reducing the variability between replicates and between alternate parameterisations of sector size, genetic dominance, and pollen and seed dispersal (Figs. 4 and 7). In contrast to pollen, which can spread resistance genes to susceptible populations but contains only half of the genetic complement of a plant; seeds contain a full set of genetic material, and seed movement therefore spreads both resistance genes and resistant individuals. The effect of GHWSd on HR evolution would be impossible to simulate accurately without the use of an integrated spatial model such as SOMER.

4.1. General recommendation for herbicide resistance modelling

Running a variety of simulations in the new SOMER model using our ‘integrated spatial modelling approach’ (accounting for every plant and weed seed within the entire field area, along with their individual age, location and resistance genetics) identified five general recommendations to consider when modelling the evolution of herbicide resistance. (1) HR modellers should seriously consider using more realistic integrated spatial models, such as the one described in this paper, rather than traditional non-spatial models, which assume spatial homogeneity. (2) Field and sector size is important, and using larger field and sector sizes has both advantages and disadvantages over smaller field and sector sizes. (3) The modeller should ensure, when using a spatial weed model, that the choice of sector size has minimal interactions with the biological characteristics of the simulated species; the trialling of alternate sector sizes is encouraged. (4) The sector size used should ensure that a significant percentage of the sub-populations initially contain no herbicide resistant seeds. (5) Pollen and harvester seed dispersal are important, and while accurate parameterisation may be difficult, their possible impact should always be considered. Pollen and seed spread parameters will also be influenced by weed species characteristics, such as flowering height, extent of pre-harvest seed drop and shattering, amount of self-pollination, and crop choice (Humston et al., 2005).

Accurately simulating the evolution of HR is made more difficult by the immense number of weed seeds found within a typical crop field. Computer simulations including the individual placement, genotype, and interactions of each weed and seed within a field is (currently) an impossible task. However, if the population is divided into sub-populations, then it is possible to simulate interactions within each sub-population in a stochastic simulation. These interactions account for each individual (seed and weed) genotype, local-scale inter-and intra-specific competition, and seed and pollen dispersal. Larger sub-populations allowed the successful simulation of individual plants and seeds across larger field areas. Therefore, the best choice of simulation field area was dependent on the type of investigation being undertaken. For example, investigations into patch dynamics yield more detail when conducted over a smaller field area, and with smaller sector sizes and finer spatial resolution. In contrast, simulations including rare resistance alleles showed reduced variability when conducted over larger field areas, because larger field areas have larger weed seed populations, and thus rare resistant genes would occur in higher numbers. Larger numbers of initially resistant individuals reduced the variability between replicates, as it allowed patch interactions and genetic combinations to occur more regularly, thus reducing small population stochastic effects. This may be useful if the aim of the study is to clearly identify average differences, but less so if the aims also include understanding variability at smaller scales. Moreover, simulating larger field sizes (up to the point where sectors became too large to mimic harvester seed dispersal) facilitated the inclusion of the dispersal of weed seeds by a grain harvester.

Typically, spatially-explicit models of field-scale weed populations use 1 m² sectors (Renton et al., 2014; Gonzalez-Diaz et al., 2015). However, SOMER allows different sector sizes to be specified. Using different-sized sub-populations (sectors from 9 m² up to 324 m²) had minimal effect on the results with current parameterisations, although care (initial background runs with alternate parameterisations) was needed to ensure parameterisation of the model was the best possible to maximise the robustness of the results. Alternative spatial divisions have been utilised in weed science, based on several ecosystem variables. For example, Garrett and Dixon (1998) based their spatial boundaries on crop positions and interaction zones, whereas Roux and Reboud (2007) considered different sizes of treated and untreated field-sized zones. In contrast, SOMER (in its current form) considers the abiotic environment to be homogeneous, and divides the field into evenly-spaced square sectors. This enables the spatially-explicit simulation of the entire field area; in a process we call ‘integrated spatial modelling’. However, certain parameter combinations of sector size and dispersal of pollen and seed generated data with higher levels of between-replicate variability, probably influenced by the probabilities of pollen and seed loss per sector (Table 4). In such cases, significantly large numbers of replicates are required to account for this variability. Additional considerations when choosing sector size are interactions with resistance gene dominance and the initial density of weed seeds (Section 3.3).

It is important for spatial simulations to begin with a high percentage of sub-populations containing no herbicide-resistant seeds. To garner the full benefits of integrated spatial modelling, sub-populations without initial resistant seeds were necessary to capture the spread of resistance, by allowing patches of resistant weeds to develop through space and time. Satisfactory results were achieved with at least 2/3 of sub-populations empty of resistance (non-resistant) in the first year, and ¾ of sub-populations non-resistant in the second year, due to local genetic drift (Table 5). Changes in the sector size that caused the proportion of non-resistant sub-populations to stay below this threshold had only a minor influence on resistance evolution predictions (Fig. 2A). The initial number of non-resistant sub-populations is influenced by sector size, weed seed density, and the initial frequency of herbicide resistant seeds. With larger sector sizes, a lower initial resistance gene frequency was needed to achieve this aim. An exception to this requirement for many initial non-resistant sub-populations could be made if resistance genes are initially at a higher frequency and evenly spread throughout the field, which is probably only relevant if we wish to model either management of existing resistance, or the spread of multiple resistance.

4.2. Limitations

It is important to acknowledge that herbicide resistance can be caused by more than one gene, and polygenic resistance can provide plants with protection from more than one herbicide group. Further work is needed to understand how dispersal and spatial structure of weed populations and genes influence the
evolution of polygenic resistance. Furthermore, weather (variation in rainfall, frosts, and wind) would affect movement of pollen and seeds within and between fields. Computational limitations when running SOMER (with spontaneous mutations) on a standard desktop computer imposes a maximum of approximately 10,000 sub-populations. This limitation meant that a smaller simulated field area of one hectare was needed to allow 1m² sectors to be implemented. The field size was limited here by the maximum number of sub-populations, although this was countered somewhat by the introduction of larger sector sizes, which, across a wide range, did not greatly affect the results. Computers that are more powerful would allow larger areas to be simulated at a fine resolution, and this may yield some benefits in prediction of resistance evolution. The variability in the initial seed distribution (SOMER currently begins with a random distribution) is also a factor affecting patch development, which could be investigated further.

5. Conclusions

Integrated spatial modelling of the spread of an herbicide-resistant annual weed predicted a slower growth in weed numbers, and a higher proportion of homozygosity, than was predicted in non-spatial modelling. Fully-dominant resistant populations exhibited more heterozygosity and evolved more rapidly than did the semi-dominant resistant populations; these differences due to dominance were also compounded at finer spatial resolutions. The parameterisation of natural seed dispersal was relatively unimportant, when compared to the pollen dispersal parameters; larger pollen dispersal distances increased resistance levels, patch size, and heterozygosity. Dispersal of 88% of seed by the harvester (as compared with no harvester seed dispersal) resulted in one less year of effective herbicide use.

The new SOMER model effectively and visually simulated the development of patches of herbicide-resistant weeds and the harvester induced spread of resistance across an annually cropped field. The new integrated spatial model has several advantages over previous models used to investigate the evolution of herbicide resistance within a population of weeds: it allows consideration to be given to localised variation in numbers (including localised extinctions), pollen and seed dispersal distances, and the effects of inadvertent grain harvester weed seed dispersal. These parameters were all identified as important in resistance evolution, in regard to both weed numbers and the evolution of an herbicide-resistant weed population.

Acknowledgements

Drs Danica Goggin and Qin Yu of AHRI at the University of Western Australia for help with this manuscript. We would also like to thank fellow modellers in Dr Renton’s study group, all at the University of Western Australia. AHRI is supported by the Grains Research and Development Corporation (GRDC).

Appendix A. Natural pollen dispersal functions

The probability that a flower is pollinated by any other plant in the simulated area is given by

\[
pollination probability_i = \frac{e^{-\alpha \frac{distance}{9.079}}}{\sum_{i=1}^{n} e^{-\alpha \frac{distance}{9.079}}}
\]

Fig. A1. Pollen dispersal curves. Fig. A1A: Fitting alternate curves using least squares to the original pollen dispersal data, which contained intraspecific competition (Knowles and Chosh 1968). For the (chosen) Weibull curve the lowest \(e = 0.0069\), for an exponential curve the lowest \(e = 0.0091\), and for a Cauchy curve the lowest \(e = 0.011\). Fig. A1B: An example of how the three pollen slope parameters altered the probability of pollination at distance. In this example there are 40 pollen source plants, progressively distant from the pollen receptive plant, with 4 positioned at each distance, 1 m through 10m. The alternate parametrisations of the pollen slope parameter are low \(a = 9.079\), medium \(a = 7.637\) and high \(a = 6.424\).
In this Weibull function $a$ is the slope parameter, $n$ is the number of flowering plants in the simulated area, and ‘distance,’ is the distance between the sector containing the pollen receptive plant and the sector containing the $i^{th}$ pollen source plant (measured using Pythagoras Theorem). From data analysis the high $a = 6.424$, generating further pollen dispersal, and the medium $a = 7.637$, generated less pollen dispersal. When these two numbers are log transformed, they become $\ln(\text{high } a) = 1.86$, and $\ln(\text{medium } a) = 2.033$. The difference between these two numbers is $2.033 - 1.86 = 0.173$ then, utilising this difference to go one step closer, $2.033 + 0.173 = 2.206$. Finally $\exp(2.206) = 9.079$. This generated very short pollen dispersal distances, with low $a = 9.079$. An example of the effect of these three slope parameters is shown in Fig. A1B.

Appendix B. Natural seed dispersal functions

The natural seed dispersal functions govern the spread of seed from one sector into the eight adjacent sectors. Natural seed dispersal within a field occurs longitudinally either within the inter-row space, or crosswise through the crop row, into the next inter-row space. Many of the weeds present at harvest are growing within the crop row, and would easily shed their seeds crosswise into the next inter-row space. In these simulations, the sector edges are not designed to line up exactly with crop rows. Therefore the rate that seed is dispersed naturally into the four side adjacent sectors (two longitudinally, and two crosswise) is assumed to be equal. Natural seed dispersal into the four corner adjacent sectors is assumed to be a later movement, from its secondary position in the four side adjacent sectors.

In our model, the probabilities of weed seed moving out of its maternal sector into each of the four directly adjacent sectors ($s$), or into each of the four corner adjacent sectors ($c$), is governed by the following functions

\[ s = \frac{w(51b^{0.5} - 2)}{200} \text{ and } c = \frac{w}{200} \]  
\[ (2) \]

where $w$ is the proportion of seed loss per square metre and $b$ is the sector area, as stated in the main text.

To highlight that these proportions vary for different sector sizes and demonstrate their equivalence for different sector sizes we can rewrite them as

\[ s_b = \frac{w(51b^{0.5} - 2)}{200} \text{ and } c_b = \frac{w}{200} \]  
\[ (B1) \]

where the subscript $b$ indicates that the proportions are for sectors of area $b$.

To demonstrate that two percent of the total seed loss from a $1 \text{ m}^2$ sector is dispersed into the four corner sectors, we can note that the total proportion of seed dispersed into the four corner sectors

\[ 4c_1 = 4\left(\frac{w}{200}\right) \text{ (from Eqn B1)} \]
\[ = 0.02w \text{ (since } b = 1) \]

To show that the total proportion of seed naturally spreading from a $1 \text{ m}^2$ sector is indeed $w$ we can note that the total proportion of seed naturally spreading from a $1 \text{ m}^2$ sector:

\[ 4s_1 + 4c_1 = 4\left(\frac{w(51b^{0.5} - 2)}{200}\right) + 4\left(\frac{w}{200}\right) \text{ (from Eqn B1)} \]
\[ = 4\left(\frac{w(51 - 2)}{200}\right) + 4\left(\frac{w}{200}\right) \text{ (since } b = 1) \]
\[ = w \frac{49}{50} + \frac{w}{50} \]
\[ = w \]

In the main text, we claimed that the functions for calculating the natural seed distribution at different sector sizes (Eq. (2)) ensure that the same amount of seed will be spread sideways per metre of sector boundary, and the same amount will be spread into the diagonal corners, thereby maintaining consistency independent of sector size (Fig. B1). To demonstrate this equivalence, we can consider a sector of area $1 \text{ m}^2$ and a sector of area $A \text{ m}^2$ and denote the number of seeds moving across one corner of these sectors as $n_{c1}$ and $n_{cA}$ respectively, and the number of seeds moving across one side of these sectors as $n_{s1}$ and $n_{sA}$ respectively. From Eqn B1, $n_{c1} = \frac{wK_1}{200}$ where $K_1$ is the amount of seed produced in the $1 \text{ m}^2$ sector. Similarly, $n_{cA} = \frac{wAK}{200A}$ where $K_A$ is the amount of seed produced in the $A \text{ m}^2$ sector. On average, $K_A = A K_1$, and so on average,

\[ n_{cA} = \frac{wAK}{200A} = \frac{wAK_1}{200A} = wK_1/200 = n_{c1} \]

and so the amount of seed moving across a corner sector is the same on average, regardless of sector size.

From Eqn B1, $n_{s1} = w K_1 \left(\frac{51 - 2}{200}\right) = w K_1/49/200$. If we consider $A \text{ m}^2$ sectors together in a square (see Fig. B1), there will be $A^{0.5}$ squares along the edge of the square, and thus the number of seeds spreading over one edge of the square will be $A^{0.5} n_{s1} + 2 \left( A^{0.5} - 1 \right) n_{c1}$ (see Fig. B1). Moreover,

\[ A^{0.5} n_{s1} + 2 \left( A^{0.5} - 1 \right) n_{c1} = A^{0.5} wK_1/49/200 + 2 \left( A^{0.5} - 1 \right) wK_1/200 \]
\[ = A^{0.5} wK_1/49/200 + 2 wK_1/200 - 2 wK_1/200 \]
\[ = K_1 \left( A^{0.5} wK_1/200 - 2 wK_1/200 \right) \]
\[ = wK_1 \left( 51wK_1/200 - 2 wK_1/200 \right) \]

\[ = 2wK_1 \]

Fig. B1. Natural seed dispersal outwards from four $1 \text{ m}^2$ sectors (on the left) and from a larger $4 \text{ m}^2$ sector (on the right).
Furthermore, from Eqn B1, \( n_{SA} = wK_A (51A^{0.5} - 2)/200A, \) so on average

\[ n_{SA} = wA K_1(51A^{0.5} - 2)/200A = wK_1(51A^{0.5} - 2)/200. \]

Thus, the number of seeds spreading over one edge of a 1 m² sectors together in a square will be the same as the number of seeds spreading over one edge of an A m² sector, and so the amount of seed moving across a sector side will be consistent for any sector size.

Appendix C. Harvester seed dispersal

As the harvester moves forward it gradually disperses the inadvertently collected weed seeds out the back of the 12 m wide harvester. The total distance of longitudinal seed dispersal is estimated to be 60 m, including 6 m backward and 54 m forward. The probabilities of longitudinal harvester seed dispersal for each 6 m distance are 0.02, 0.22, 0.26, 0.23, 0.1, 0.07, 0.05, 0.03, 0.01 and 0.01 (scaled up from measurements in Blanco-Moreno et al. [2004]). For sectors that are less than 6 m wide these probabilities were shared equally within the 6 m, and for sectors that are more than 6 m wide the probabilities were shared proportionally among neighbouring sectors, so that the dispersal pattern remained similar. Seed is spread evenly within each 12 m wide crosswise row of sectors, extending across the width of harvester. Seed to be spread within each crosswise row is mixed, prior to dispersal into the individual sectors within each 12 m wide crosswise row. The results are shown in Fig. C1.

Appendix A. Supplementary data

Supplementary data associated with this article can be found, in the online version, at http://dx.doi.org/10.1016/j.ecolmodel.2017.08.002.

References


