gc_memo default simulation parameters

Infection schedule, antigen and limiting factor presence

symbol	default value	meaning	source / reason
t_{vacc}	[0, 28, 56]	Vaccination schedule in days	CHMI trial underlying this work (Mordmüller et al., 2017)
τ_{decay}	2 days	Time constant of exponential Ag decay/removal in the system	(Mandel et al., 1980)
p_{base}	0.005	Base activation probability per free B cell and timestep	choice leading to 10% activation
$t_{GC,max}$	day 7	Day until which the GC stays at maximum size	onset of *Pf* blood stage (Keitany et al., 2016)
$\tau_{GC\ decay}$	10 days, *varies*	Time constant of exponential limiting factor decay after $t_{GC,max}$	set to reduce GC size faster than normal (Wittenbrink et al., 2011; Weisel et al., 2016; Gulbranson et al., 1996) due to blood stage antigens (Keitany et al., 2016)

GC dynamics

symbol	default value	meaning	source / reason
t_{init}	3 days	Time needed by B cells to become fully activated and migrate to the follicle to form a GC after initial antigenic contact	(De Silva et al., 2015)
t_{AID}	3 days	Time needed for cells having newly joined the GC before they start acquiring mutations during divisions	(Kleinstein et al., 2003)
t_{help}	2 hours	Time that selected B cells receive survival signals before deciding to divide or differentiate	order of (Allen et al., 2007a) (several contacts of 10-60 minutes)
n_{div}	2	number of divisions B cells undergo following selection	mean in (Gitlin et al., 2014)
t_{div}	8 hours	Time needed for cell division in the GC after having received survival signal	(Allen et al, 2007b)
t_{diff}	8 hours	Time needed for differentiation into a memory cell after having received survival signal	chosen to match t_{div}
$t_{life,\ GC}$	8 hours	Maximum survival time of GC cells in the waiting area	choice with minor effect on results
$t_{life,\ naive}$	14 days	Lifetime of naïve cells that have not been activated; new naïve cells are continuously introduced into the simulation to keep up the poolsize n_{naive}	(Macallan et al., 2012)
r	0.9	Fraction of cells choosing to divide and recycle instead of leaving as a differentiated cell after receiving survival signal	(Meyer-Hermann et al., 2012)

p_{PC}	0.5	Fraction of exported cells that are of plasma cell phenotype, 1-p_{PC} are exported as memory; since plasma cells are not modeled explicitly, the cells in question are removed from the system	(Chaudhury et al., 2014)

Binding model & mutations

symbol	default value	meaning	source / reason
n_{key}	[1 … 15]	Number of residues jointly determining affinity towards a given epitope sequence	text
n_V	220	Combined length of the V_H and V_L segments	
b^{thr}	0.6	Binding threshold in normalized energy units	text
K_D^{thr}	10^{-5} M	Corresponding binding threshold as dissociation constant	(Batista et al., 1998; Childs et al., 2015)
b^{top}	1	Maximum binding strength in normalized energy units	text
K_D^{top}	10^{-9} M	Corresponding maximum binding strength as dissociation constant	(Batista et al., 1998; Childs et al., 2015)
p_{err}	0.003	Error probability per codon and division	(Li et al., 2004)
p_{death}	0.5	Probability that a replacement mutation in a residue relevant for stability leads to a non-functional Ab (and hence cell death)	(Kleinstein et al., 2003)
p_{block}	0.55	Probability that a mutation in a non-key residue results in blocking of affinity maturation	mean of values given in (Kleinstein et al., 2003)

Simulation size

symbol	default value	meaning	source / reason
n_{GC}	50, *varies*	Number of individual GCs in the system	text, weak affect on results
n_{LF}	25, *varies*	Number of limiting factors (T_{FH} cells) per GC	leads to GCs of 500 cells in steady state, in range of (Wittenbrink et al., 2010)
n_{naive}	1000, *varies*	Steady state number of potentially binding free naïve cells per GC	estimation: (B cells in mouse (Matsumoto et al., 1995)) * (precursor frequency (Perelson et al., 1979))/n_{GC} = 10^9*10^{-4}*10^{-2} = O(10^3)
$n_{freemem}$	100	Number of binding free memory cells from former infections per GC at t=0	(Perez-Andres et al., 2010) and text
t_{step}	2 hours	Simulation timestep	chosen to match smallest simulated time unit (t_{help})