Supporting Information for *Size-dependent clustering in phytoplankton communities in a 3D environment* by C. Picoche & F. Barraquand.

S1 Pair correlation function in the Brownian Bug Model

We show here how to compute the monospecific pair correlation function using the Brownian Bug Model. In 3 dimensions, when the growth rate λ is the same as the mortality rate μ, the pair density $G(r)$ (where $G(r) = C^2 g(r)$) is a solution of eq. 1 (see Young et al. and Picoche et al. for a detailed explanation).

$$\frac{\partial G}{\partial t} = \frac{2D}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial G}{\partial r}\right) + \frac{\gamma}{r^2}\frac{\partial}{\partial r}\left(r^4\frac{\partial G}{\partial r}\right) + 2\lambda C\delta(\boldsymbol{r}) \tag{1}$$

In the presence of advection ($\gamma \neq 0$), a steady-state solution can be found.

$$\begin{aligned}
0 &= \frac{2D}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial G}{\partial r}\right) + \frac{\gamma}{r^2}\frac{\partial}{\partial r}\left(r^4\frac{\partial G}{\partial r}\right) + 2\lambda C\delta(\boldsymbol{r}) \\
\Leftrightarrow 0 &= 4\pi r^2\left(\frac{2D}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial G}{\partial r}\right) + \frac{\gamma}{r^2}\frac{\partial}{\partial r}\left(r^4\frac{\partial G}{\partial r}\right) + 2\lambda C\delta(\boldsymbol{r})\right) \\
\Leftrightarrow 0 &= 4\pi\left(2D\frac{\partial}{\partial r}\left(r^2\frac{\partial G}{\partial r}\right) + \gamma\frac{\partial}{\partial r}\left(r^4\frac{\partial G}{\partial r}\right)\right) + 4\pi r^2 2\lambda C\delta(\boldsymbol{r})
\end{aligned} \tag{2}$$

We can then integrate Eq. (1) over a small sphere centered on a particle, with radius ρ. Let us first note that

$$\begin{aligned}
\int_{\mathbb{R}^3}\delta(\boldsymbol{r})d^3\boldsymbol{r} &= 1 \\
\Leftrightarrow \int_0^{2\pi}\int_0^{\pi}\int_0^{\rho}\delta(\boldsymbol{r}')r'^2\sin(\phi) \quad dr' \quad d\phi d\theta &= 1 \\
\Leftrightarrow 4\pi\int_0^{\rho}\delta(\boldsymbol{r}')r'^2 dr' &= 1
\end{aligned} \tag{3}$$

Using Eq. (2) and (3),

$$\begin{aligned}
0 &= 4\pi\left(2D\rho^2\frac{\partial G}{\partial r} + \gamma\rho^4\frac{\partial G}{\partial r}\right) + 2\lambda C \\
\Leftrightarrow \frac{\partial G}{\partial r} &= -\frac{1}{4\pi}\frac{2\lambda C}{2D\rho^2 + \gamma\rho^4}
\end{aligned} \tag{4}$$

We can integrate between ρ and ∞, knowing that $G(\infty) = C^2$.

$$C^2 - G(\rho) = -\frac{1}{4\pi}\int_{\rho}^{\infty}\frac{2\lambda C}{2Dr^2 + \gamma r^4}dr \tag{5}$$

$$\Leftrightarrow G(\rho) = C^2 + \lambda C\frac{\sqrt{\gamma}\rho\arctan\left(\frac{\sqrt{\gamma}\rho}{\sqrt{2D}}\right) + \sqrt{2D}}{2^{5/2}D^{3/2}\pi\rho} \tag{6}$$

Finally, the pair correlation function $g = G/C^2$ is defined as

$$g = \frac{\lambda}{4\pi C}\left(\frac{\sqrt{\gamma}\arctan\left(\frac{\sqrt{\gamma}\rho}{\sqrt{2D}}\right)}{2^{3/2}D^{3/2}} + \frac{1}{2Dr} - \frac{\pi\sqrt{\gamma}}{2^{5/2}D^{3/2}}\right) + 1 \tag{7}$$

S2 Computation of the (cross-)pair correlation function and dominance index

S2.1 Parameters for the computation

The algorithm for pcf computation was mostly taken from the function `pcf3est` in spatstat 2.2-0 and adapted to also compute multispecific pcf. This function was first tested on known distributions (Poisson and Thomas distributions, see Fig. S1). When using the Thomas distribution, characterized by a stronger clustering at smaller scales, we found that the original bandwidth value used in spatstat, $\delta = 0.26/C^{1/3}$, could not adapt to small scale clusters and we had to switch to a fixed, smaller value of δ (Fig. S2).

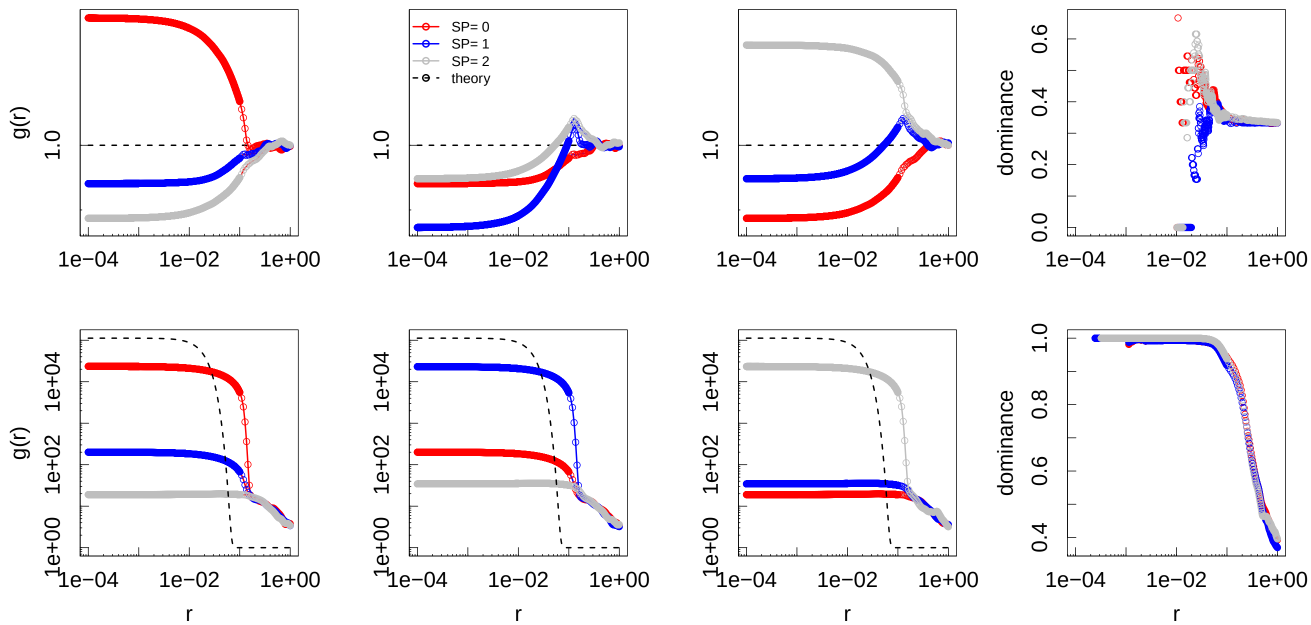

Figure S1: Monospecific pcf and dominance for Poisson and Thomas distributions for 3 species with the same concentration ($\approx$ 10 000 C/L). Theoretical values of the pcf are indicated by the dashed line.

To compute the pcf with the Brownian Bug Model, we looked for a bandwidth that could get the monospecific pcf closer to its theoretical counterpart, assuming that it would be also adapted to the multispecific pcf. We found that $\delta = 10^{-5}$ could give consistent values for both diatoms and nanophytoplankton particles (Fig. S3).

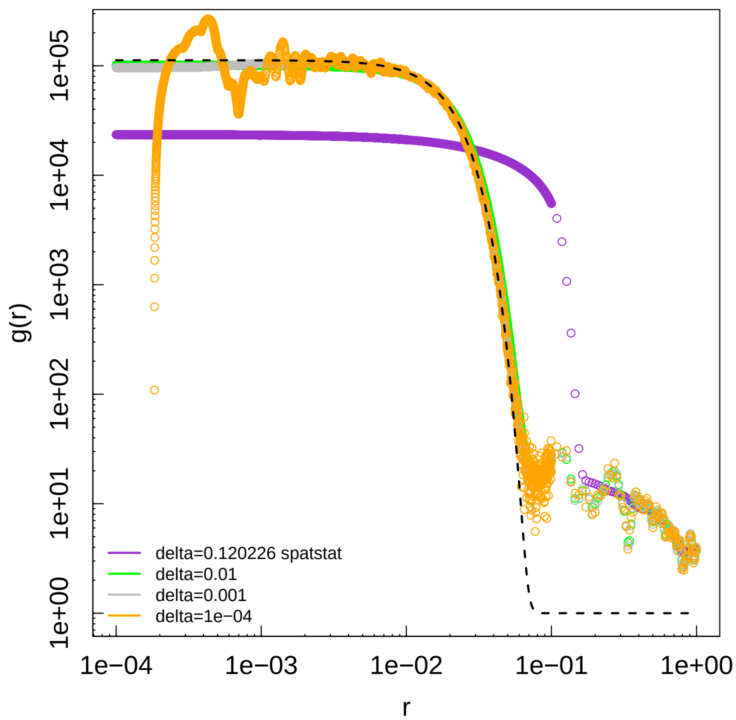

Figure S2: Monospecific pcf computed for the Thomas distribution for 3 species, with different values of the bandwidth. The dashed line indicates the theoretical pcf.

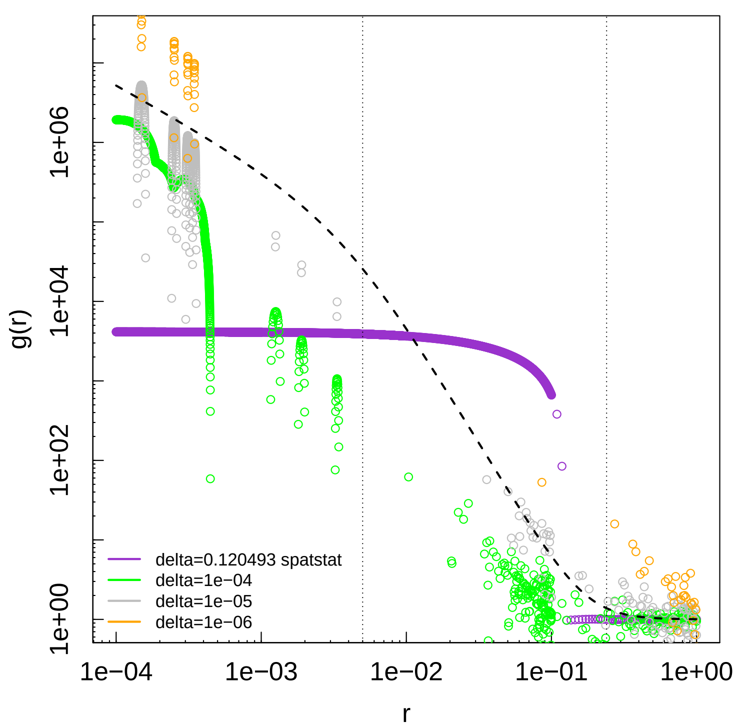

Figure S3: Monospecific pcf computed for the Brownian bug model with diatom-like particles, after 1000 time steps, with different values of the bandwidth. The dashed line indicates the theoretical pcf.

S2.2 Mono- and multispecific pcf in the Brownian Bug Model

We show here the values of mono- and multispecific pcf for diatoms and nanophytoplankton particles.

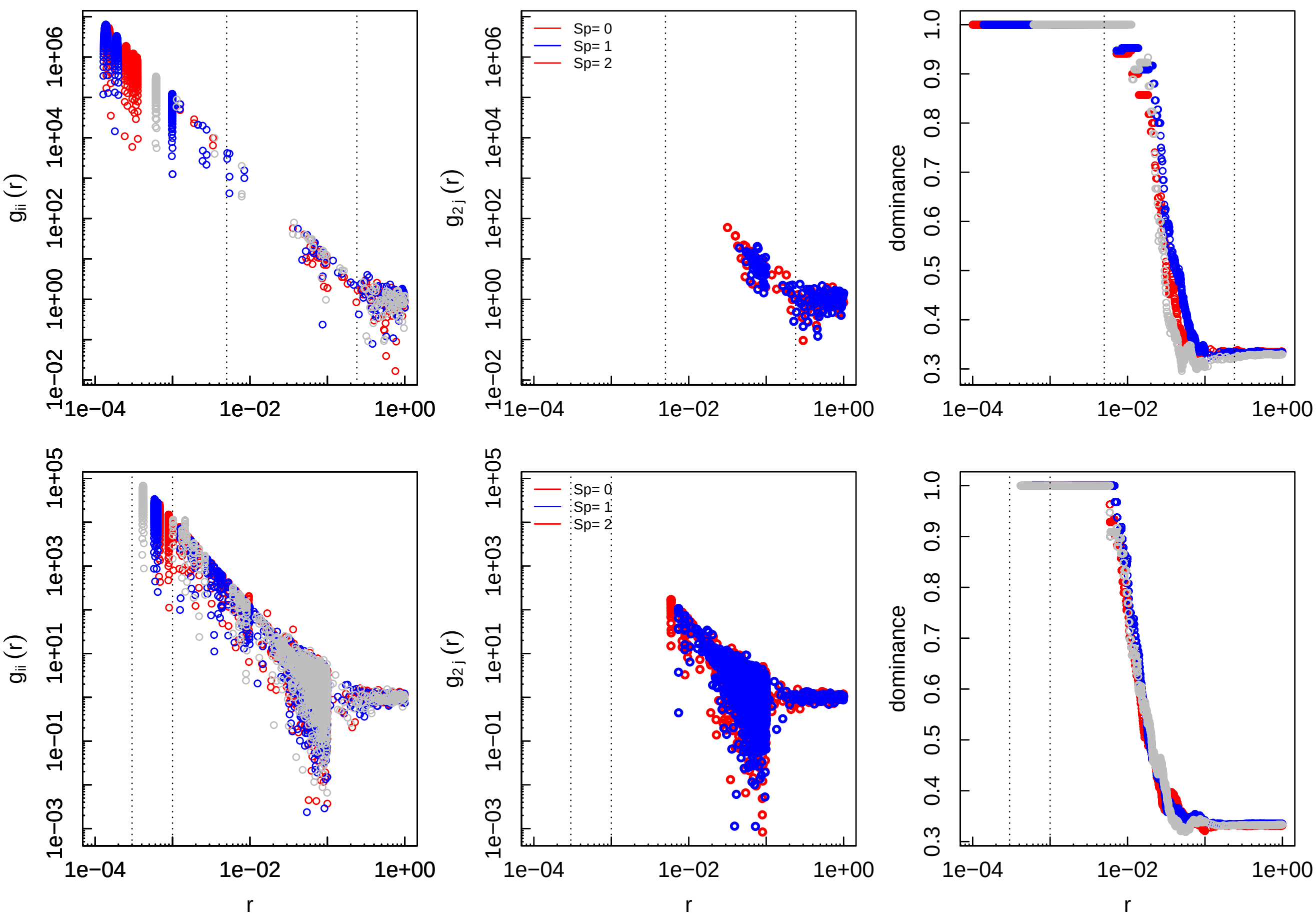

Figure S4: Monospecific (left), multispecific (middle) and dominance (right) for diatoms (top) and nanophytoplankton (bottom), after 1000 time steps. Dotted lines indicate the assumed limits for interactions between particles.