Supplementary Material for Macromolecules

Nanorod diffusion in polymer nanocomposites by molecular dynamics simulations

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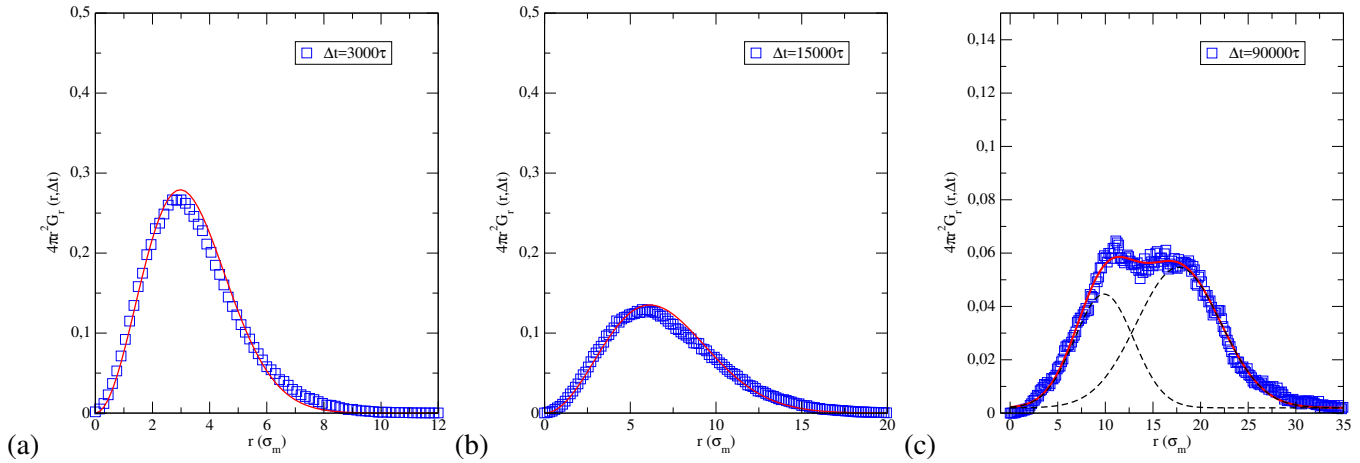

FIG. S1: van Hove function $G_s(r, \Delta t)$ for nanorods in nanocomposite, nanorod diameter $D = 3$, $AR = 8$ polymer matrix $N = 10$, at three different Δt. Blue symbols are data from the simulations, and solid lines are fitting of Equation 9 in the first two panels (a)+(b) for $\Delta t \leq 15\tau$, while the right panel (c) for larger time interval $\Delta t = 90\tau$ can only be fitted by a superposition of two Gaussians. The individual contributions are shown by black dashed lines.

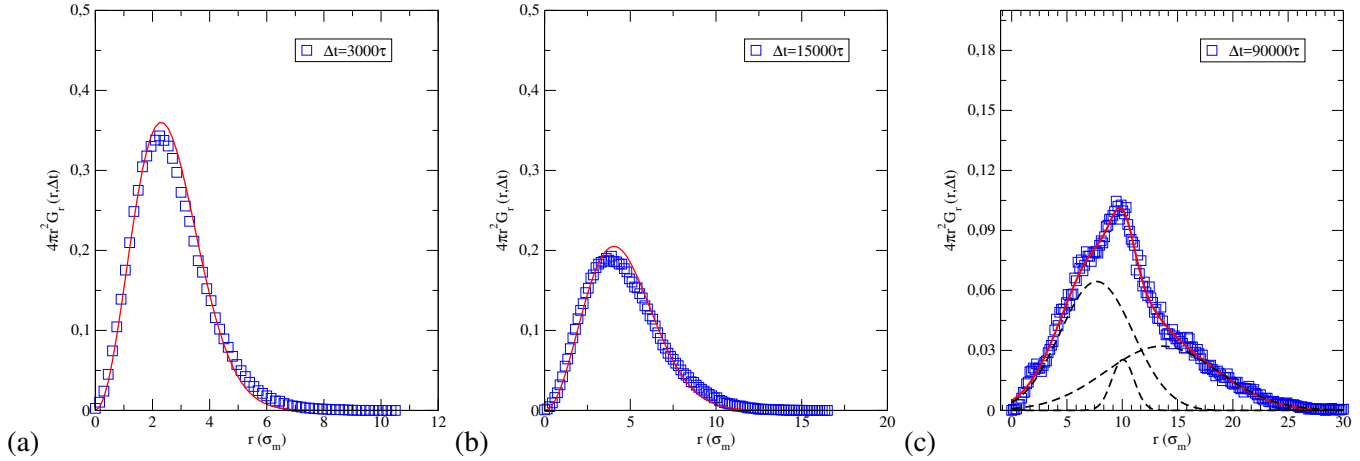

FIG. S2: van Hove function $G_s(r, \Delta t)$ for nanorods in nanocomposite, nanorod diameter $D = 3$, $AR = 8$ polymer matrix $N = 20$, at three different Δt. Blue symbols are data from the simulations, and solid lines are fitting of Equation 9 in the first two panels (a)+(b) for $\Delta t \leq 15\tau$, while the right panel (c) for larger time interval $\Delta t = 90\tau$ can only be fitted by a superposition of three Gaussians. The individual contributions are shown by black dashed lines.

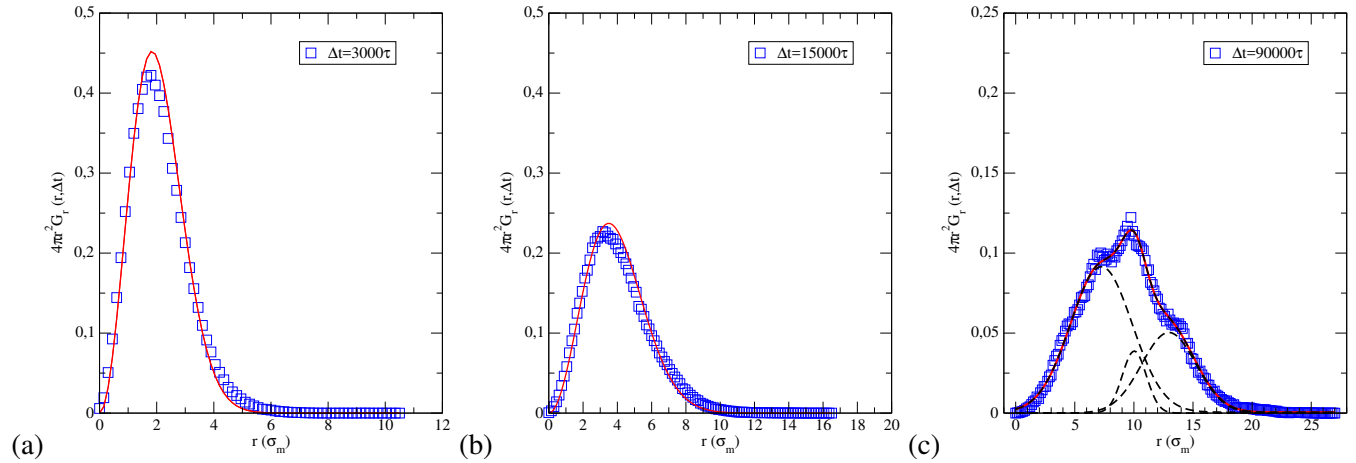

FIG. S3: van Hove function $G_s(r, \Delta t)$ for nanorods in nanocomposite, nanorod diameter $D = 3$, $AR = 8$ polymer matrix $N = 50$, at three different Δt. Blue symbols are data from the simulations, and solid lines are fitting of Equation 9 in the first two panels (a)+(b) for $\Delta t \leq 15\tau$, while the right panel (c) for larger time interval $\Delta t = 90\tau$ can only be fitted by a superposition of three Gaussians. The individual contributions are shown by black dashed lines.

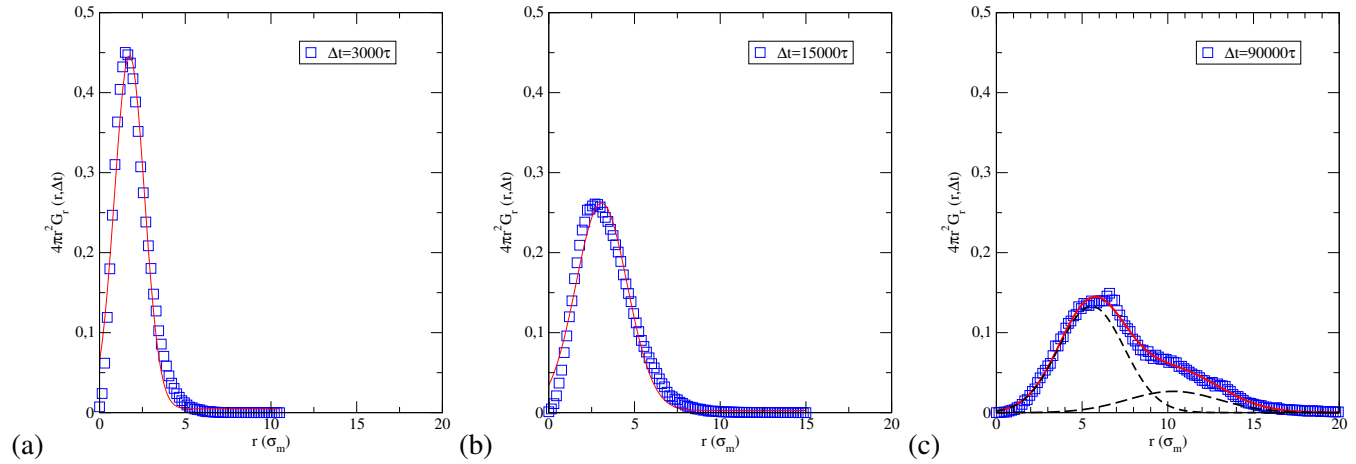

FIG. S4: van Hove function $G_s(r, \Delta t)$ for nanorods in nanocomposite, nanorod diameter $D = 3$, $AR = 8$ polymer matrix $N = 100$, at three different Δt. Blue symbols are data from the simulations, and solid lines are fitting of Equation 9 in the first two panels (a)+(b) for $\Delta t \leq 15\tau$, while the right panel (c) for larger time interval $\Delta t = 90\tau$ can only be fitted by a superposition of two Gaussians. The individual contributions are shown by black dashed lines.

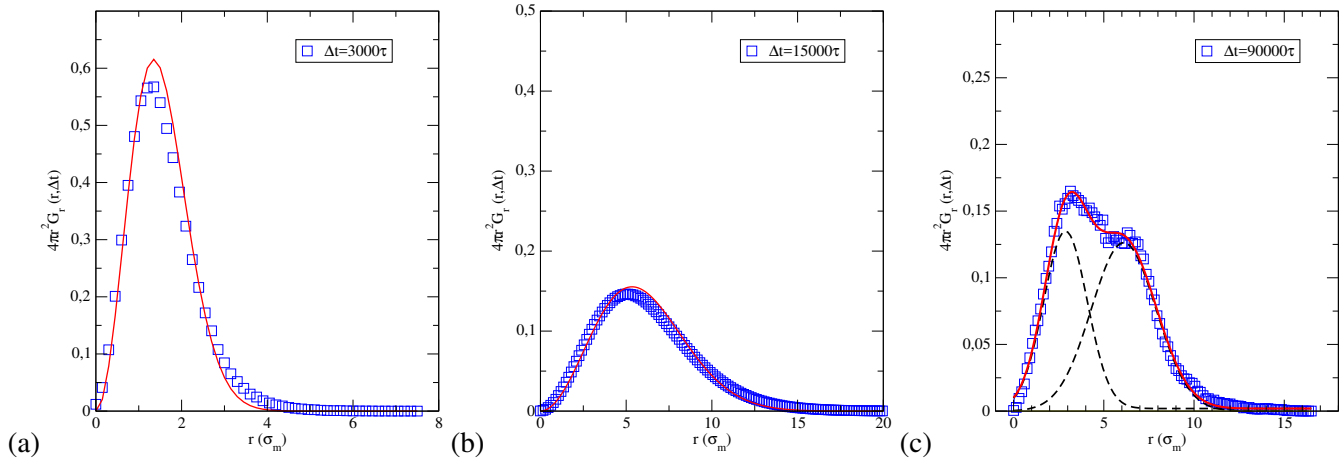

FIG. S5: van Hove function $G_s(r, \Delta t)$ for nanorods in nanocomposite, nanorod diameter $D = 4$,$AR = 8$ polymer matrix $N = 100$, at three different Δt. Blue symbols are data from the simulations, and solid lines are fitting of Equation 9 in the first two panels (a)+(b) for $\Delta t \leq 15\tau$, while the right panel (c) for larger time interval $\Delta t = 90\tau$ can only be fitted by a superposition of two Gaussians. The individual contributions are shown by black dashed lines.

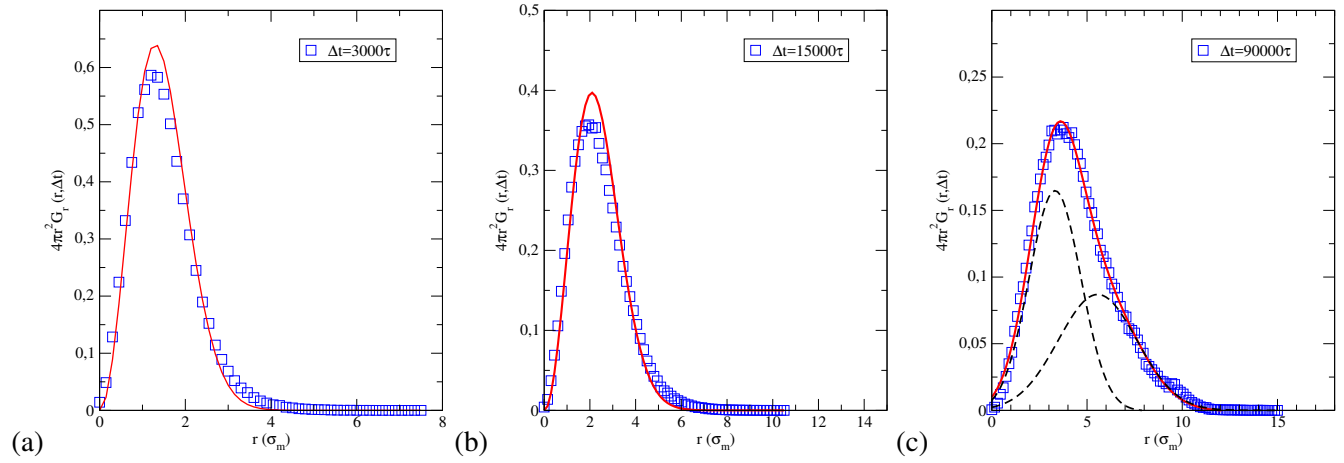

FIG. S6: van Hove function $G_s(r, \Delta t)$ for nanorods in nanocomposite, nanorod diameter $D = 4$,$AR = 8$ polymer matrix $N = 400$, at three different Δt. Blue symbols are data from the simulations, and solid lines are fitting of Equation 9 in the first two panels (a)+(b) for $\Delta t \leq 15\tau$, while the right panel (c) for larger time interval $\Delta t = 90\tau$ can only be fitted by a superposition of two Gaussians. The individual contributions are shown by black dashed lines.

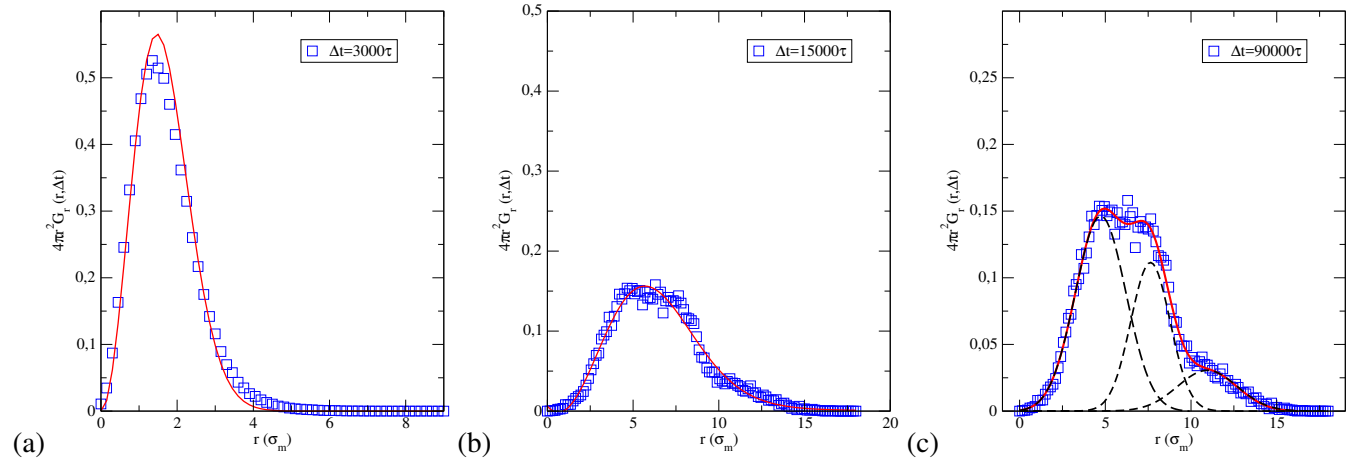

FIG. S7: van Hove function $G_s(r, \Delta t)$ for nanorods in nanocomposite, nanorod diameter $D = 4$, $AR = 8$, polymer matrix $N = 50$, at three different Δt. Blue symbols are data from the simulations, and solid lines are fitting of Equation 9 in the first two panels (a)+(b) for $\Delta t \leq 15\tau$, while the right panel (c) for larger time interval $\Delta t = 90\tau$ can only be fitted by a superposition of three Gaussians. The individual contributions are shown by black dashed lines.

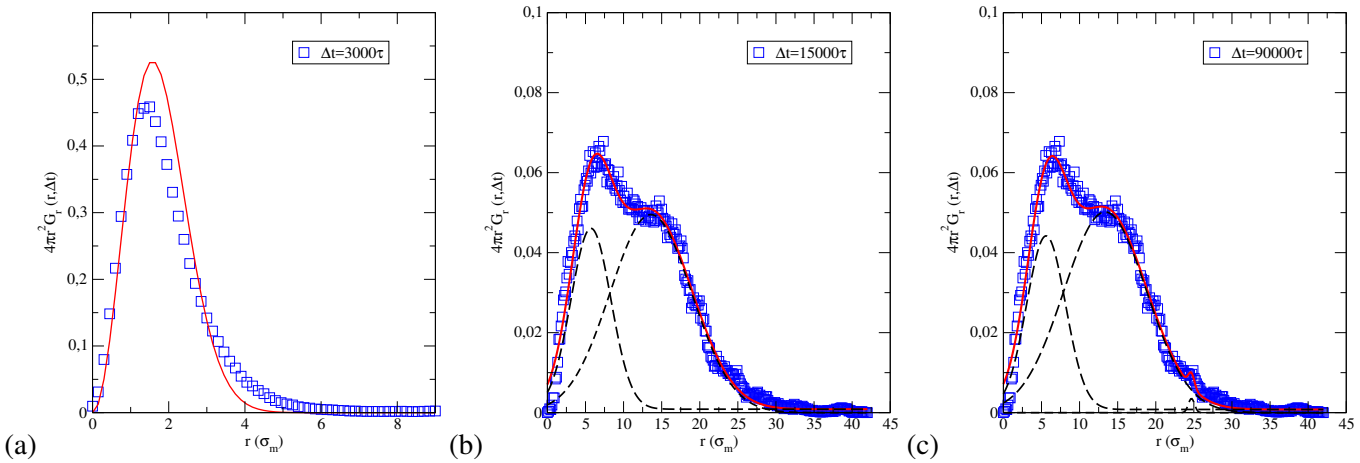

FIG. S8: van Hove function $G_s(r, \Delta t)$ for nanorods in nanocomposite, nanorod diameter $D = 4$, $AR = 8$ polymer matrix $N = 20$, at three different Δt. Blue symbols are data from the simulations, and solid lines are fitting of Equation 9 in the first panel (a) for $\Delta t = 3\tau$, while the other two panels (b)+(c) for larger time interval $\Delta t = 15, 90\tau$ can only be fitted by a superposition of two Gaussians. The individual contributions are shown by black dashed lines.

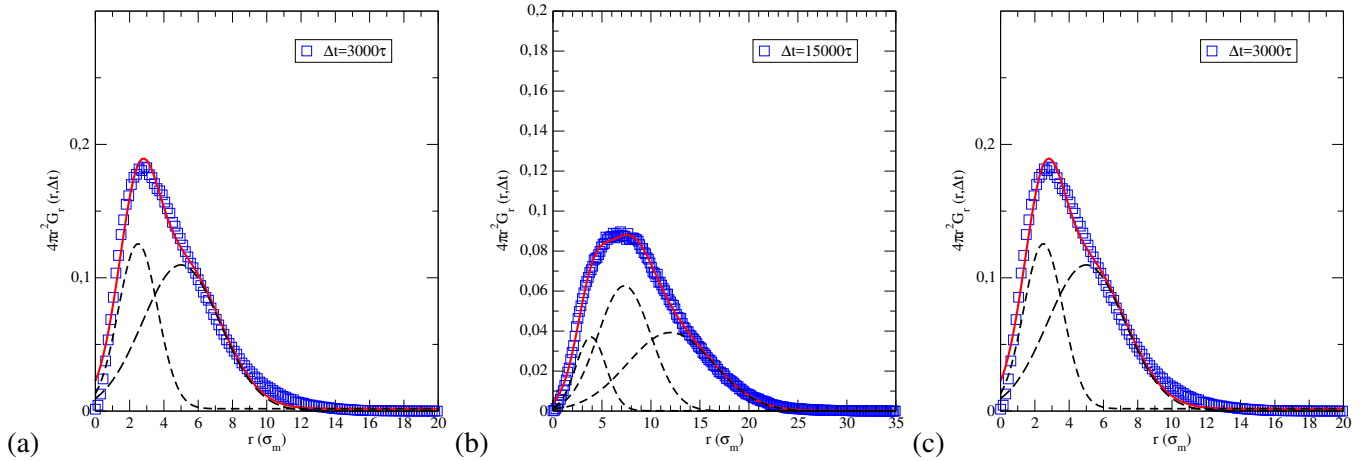

FIG. S9: van Hove function $G_s(r, \Delta t)$ for nanorods in nanocomposite, nanorod diameter $D = 2$, $AR = 8$ polymer matrix $N = 100$, at three different Δt. Blue symbols are data from the simulations, and solid lines are fitting by a superposition of two or three Gaussians. The individual contributions are shown by black dashed lines.

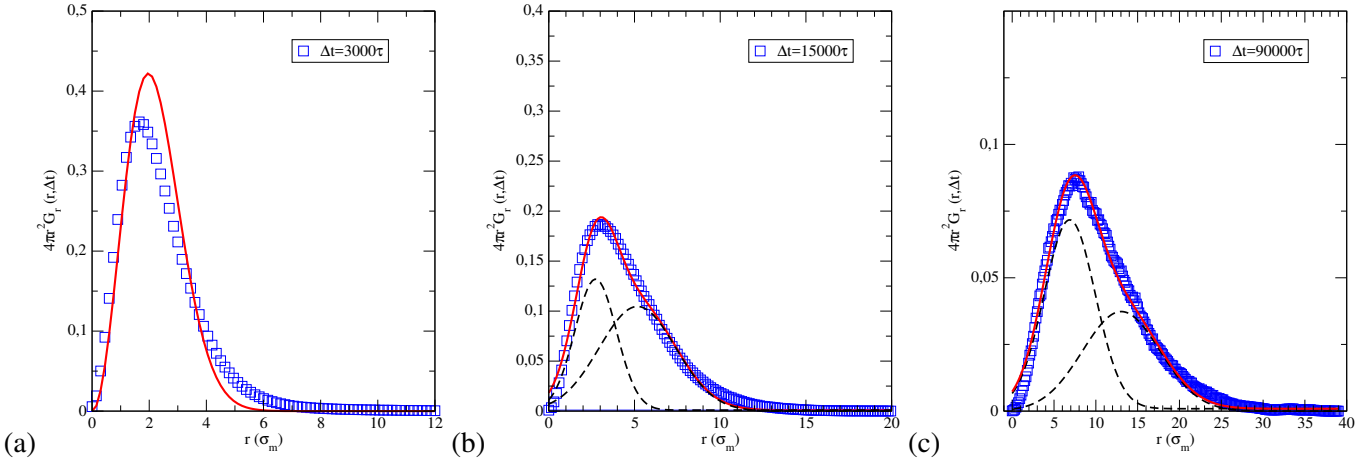

FIG. S10: van Hove function $G_s(r, \Delta t)$ for nanorods in nanocomposite, nanorod diameter $D = 1$, $AR = 16$ polymer matrix $N = 50$, at three different Δt. Blue symbols are data from the simulations, and solid lines are fitting of Equation 9 in the first panel (a) for $\Delta t = 3\tau$, while the other 2 panels (b)+(c) for larger time intervals $\Delta t = 15, 90\tau$ can only be fitted by a superposition of two Gaussians. The individual contributions are shown by black dashed lines.

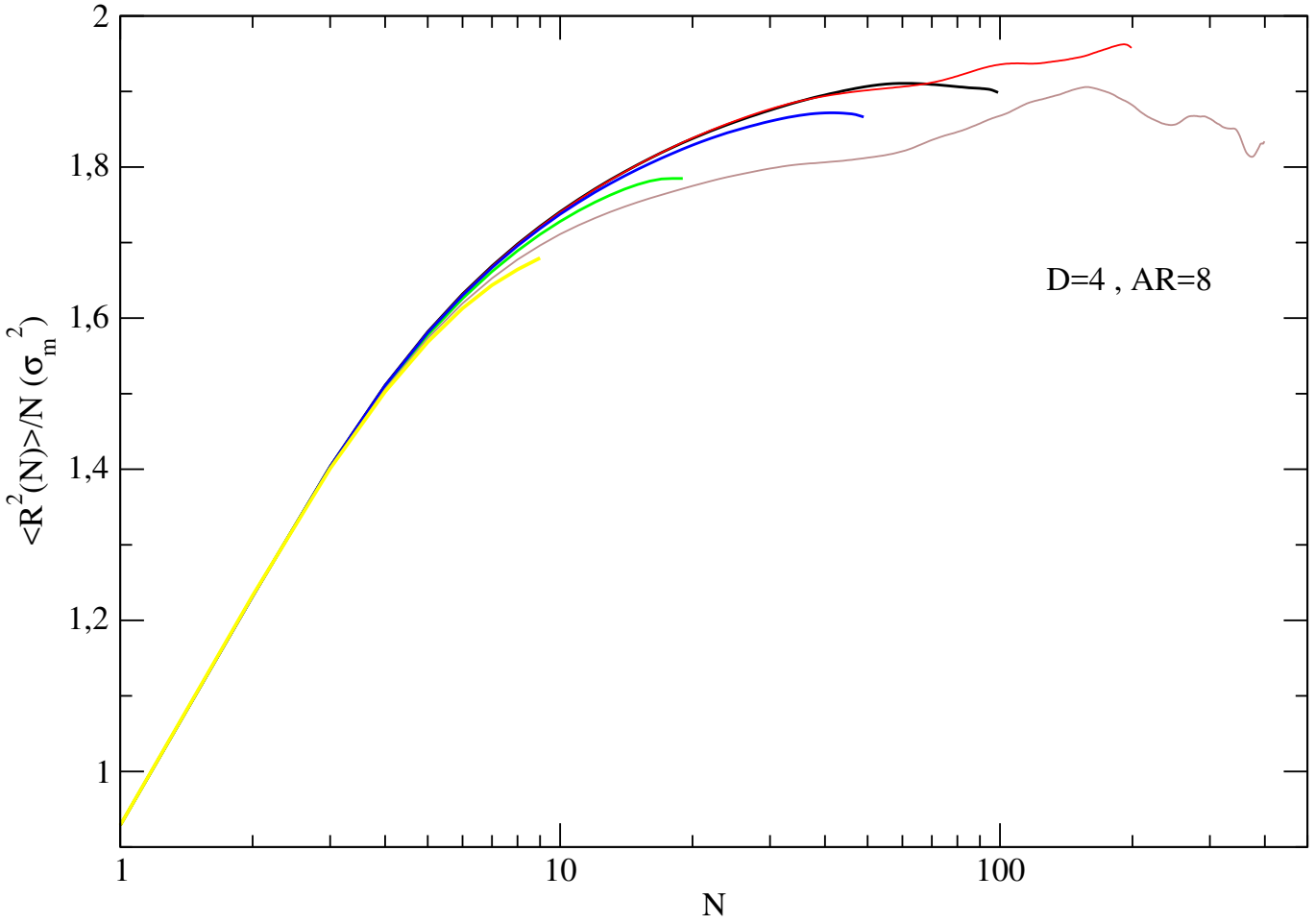

FIG. S11: Mean square internal distances for polymers in nanocomposites containing nanorods ($D = 4$) with $AR = 8$.

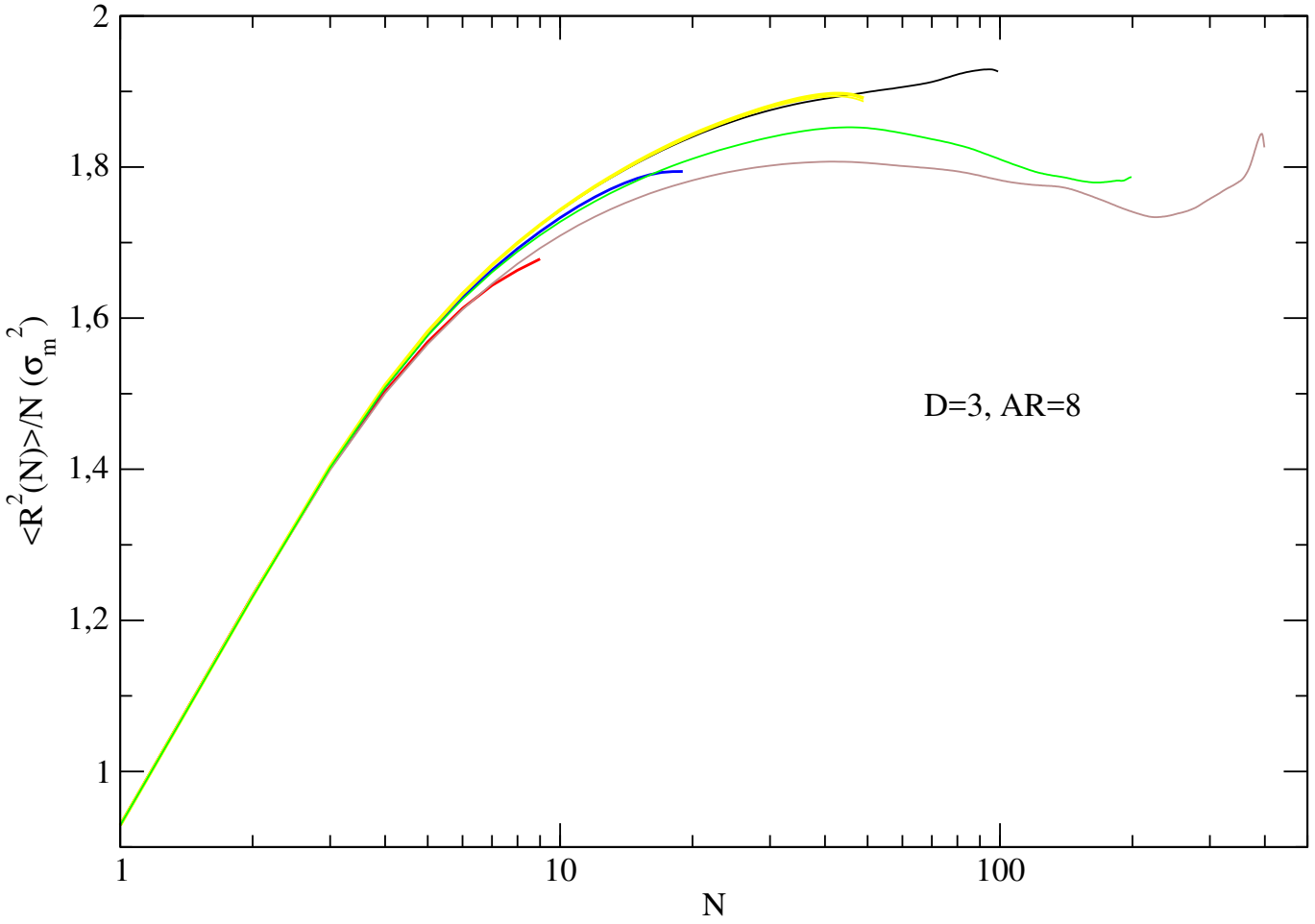

FIG. S12: Mean square internal distances for polymers in nanocomposites containing nanorods ($D = 3$) with $AR = 8$.

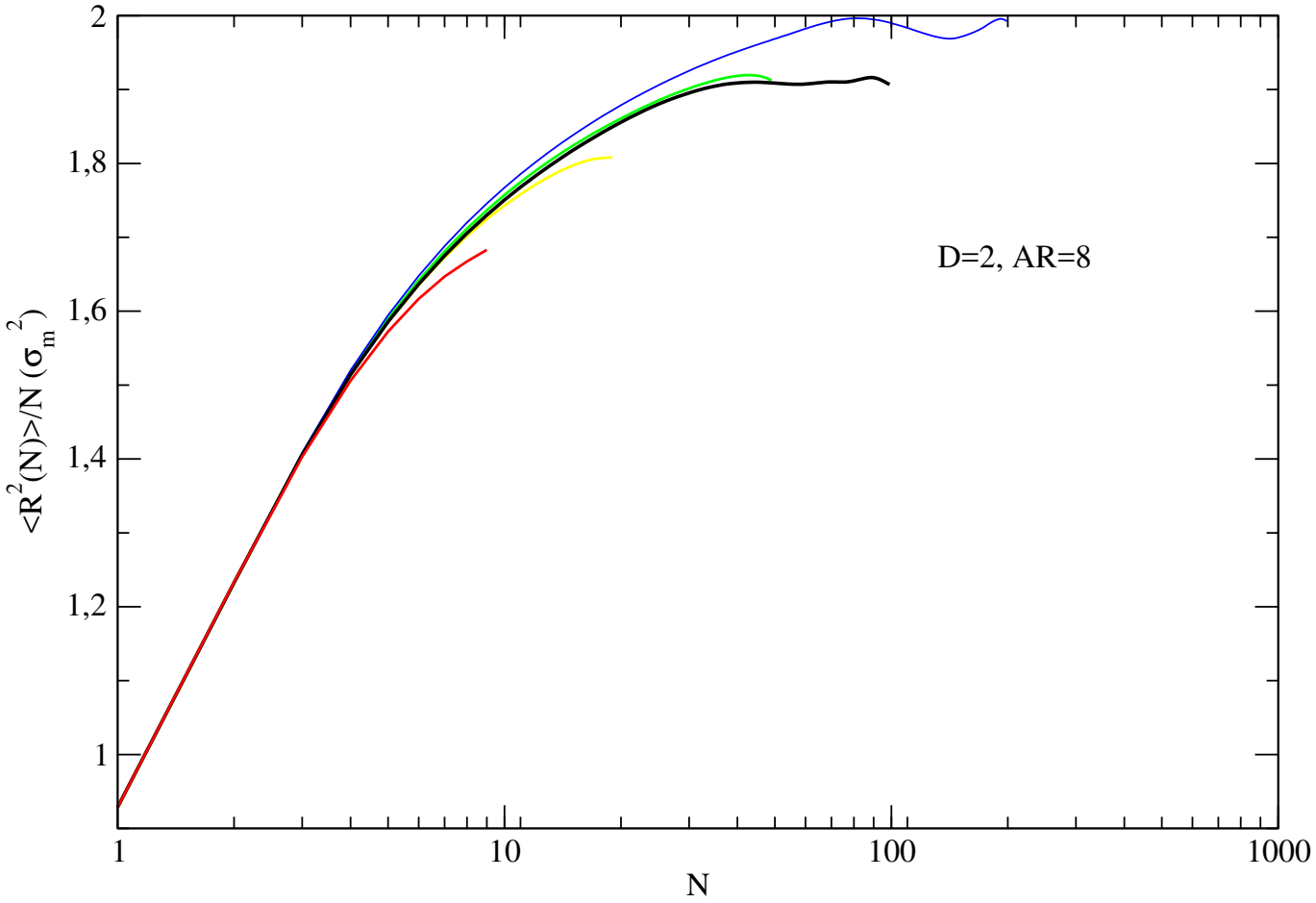

FIG. S13: Mean square internal distances for polymers in nanocomposites containing nanorods ($D = 2$) with $AR = 8$.

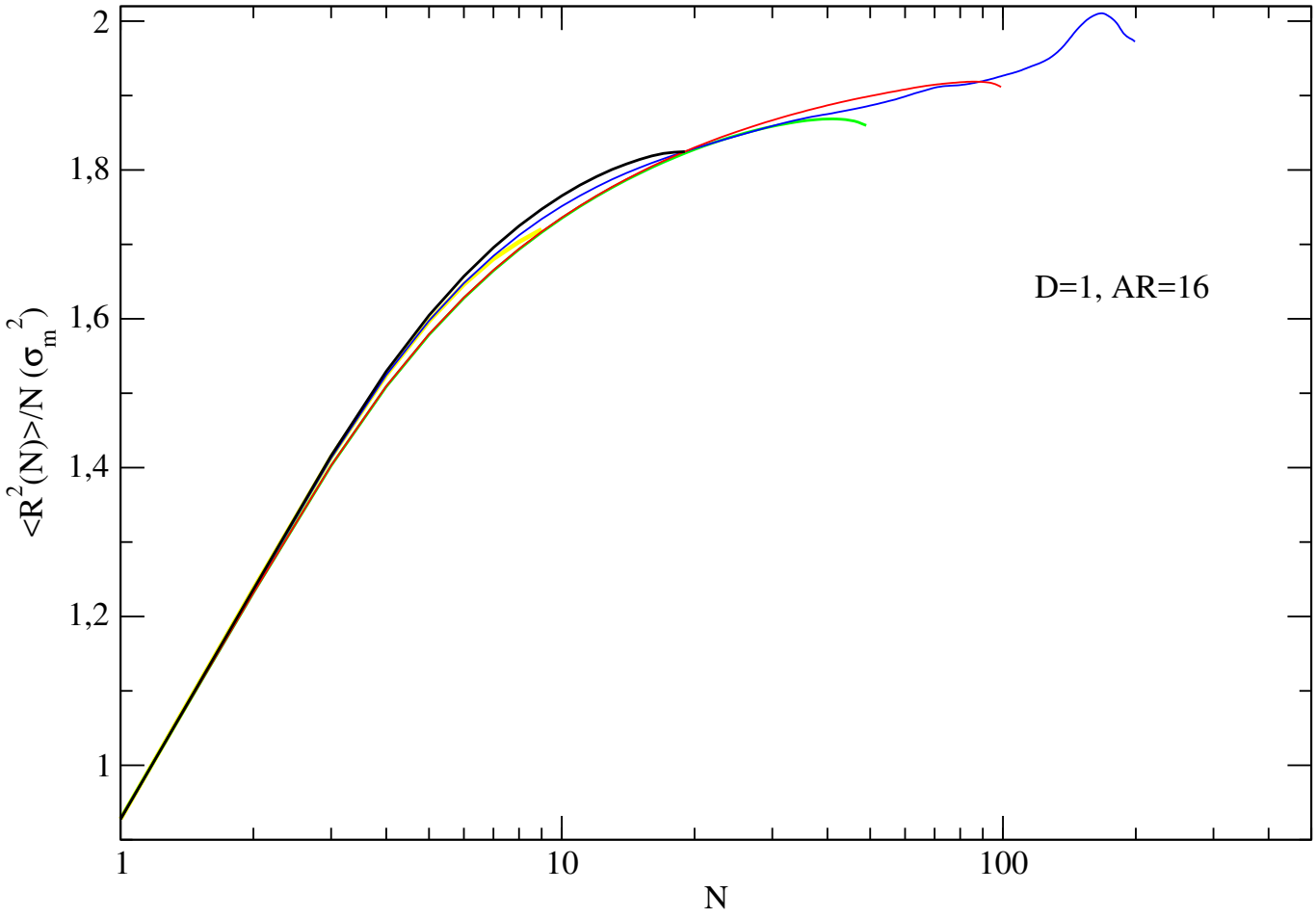

FIG. S14: Mean square internal distances for polymers in nanocomposites containing nanorods ($D = 1$) with $AR = 16$.

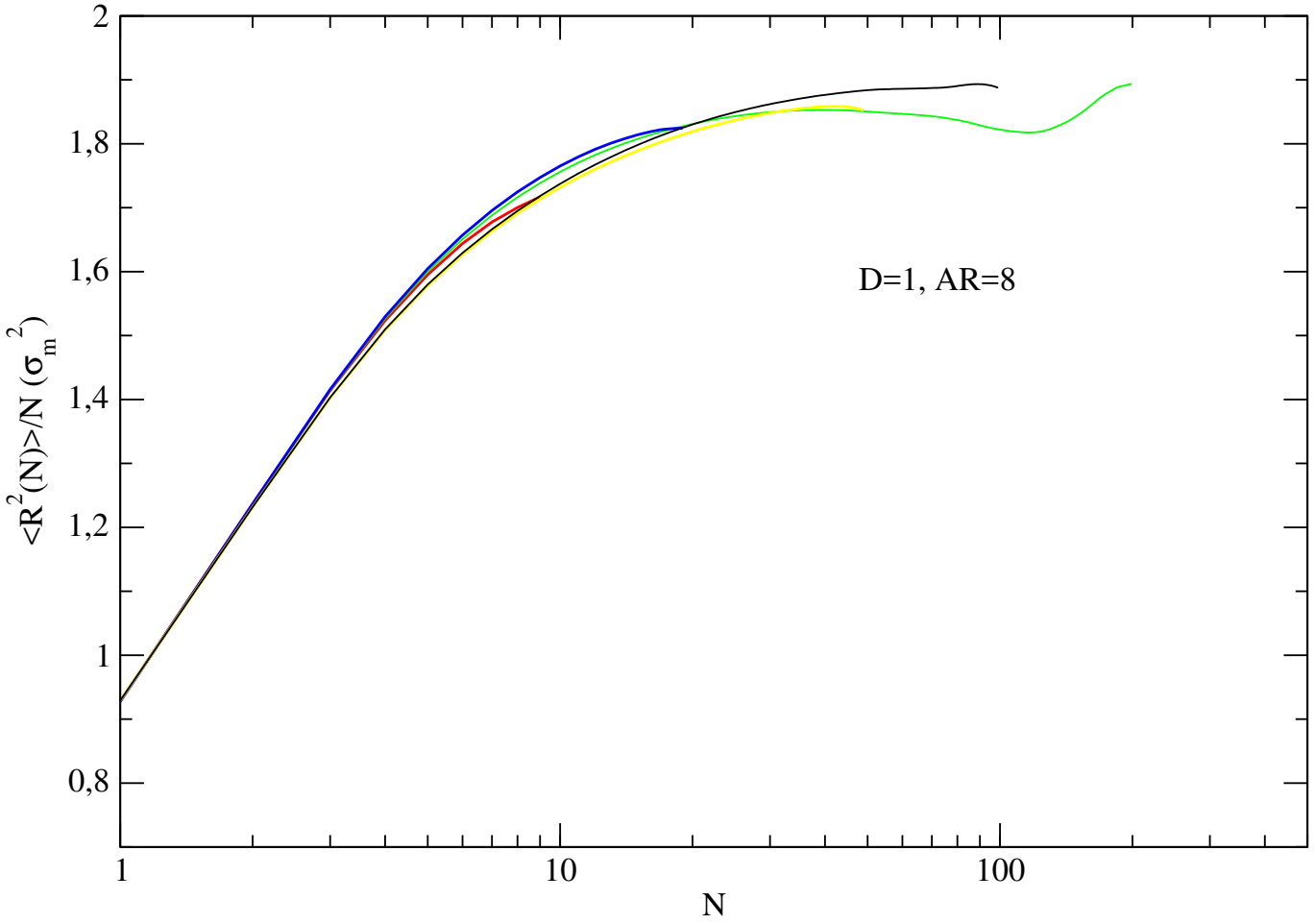

FIG. S15: Mean square internal distances for polymers in nanocomposites containing nanorods ($D = 1$) with $AR = 8$.