I. Supplementary Figures

Figure S1: Heterogeneity in Stemness, EMT potential and Biophysical characteristics of human breast cancer cells. (A-D) tSNE showing patient Id (A), expression levels of Biophysical properties (B), Stemness (C) and EMT score (D) for each cell in the breast cancer dataset GSE75688. (E-F) Plots of cellular-level enrichment score of Stemness and EMT potential compared to BiophysicalScore.
Figure S2: Expression levels of biophysical markers, EMT markers and Stemness markers in MCF7 cell line scRNA-Seq dataset (GSE115869, 1000 cells) and MDA-MB-231 scRNA-Seq dataset (GSE124989, 121 cells).
Figure S3. (A) Initial radial distribution ($r$) of cell size and deformability cells within the heterogeneous cluster for different values of $J_{cc}$. (B) Close-up of simulation lattice showing possible interactions between cell pixels, ECM pixels and fluid pixels. (C) Fluctuations in cell size of individual cells (each colour represents a different cell) over the course of the simulations. (D) Representative random cell trajectories of cells for the case of (i) homogeneous cell size and deformability and (ii) heterogeneous cell size and deformability. Grey circles depict the position of the cell cluster at $t = 0$. (E) Quantification of population-averaged cell translocation ($\bar{D}$) for the case of (i) homogeneous cell size and heterogeneity in deformability (ii) heterogeneous cell size with homogenous deformability and (iii) heterogeneity in both cell size and deformability for three different values of $J_{cc}$. Error bars: ± Standard Error of Mean (SEM). Statistical significance was assessed by $t$ test (ns: not significant, **: $p < 0.01$, ***: $p < 0.001$, ****: $p < 0.0001$).
Figure S4. Representative snaps of migration of heterogeneous cluster in the presence of a stable chemokine gradient of varying chemotactic strength ($\mu = \{250, 500, 1000, 2000\}$) and different values of $J_{cc}$. Simulations were run for 2010 MCS for $\mu \in \{250, 1000\}$. For $\mu = 2000$, simulations were run till $t = t^*$ as indicated in each case.
**Figure S5:** (A) Quantification of $\delta$ for the case of (i) homogeneous cell size and heterogeneity in deformability (ii) heterogeneous cell size with homogenous deformability, and (iii) heterogeneity in both cell size and deformability for three different values of $J_{cc}$. Error bars: ± Standard Error of Mean (SEM). Statistical significance was assessed by $t$ test (ns: not significant, *: $p < 0.05$, **: $p < 0.01$, ****: $p < 0.0001$). (B) Plot of average number of neighbour changes every 10 MCS for cells for three different values of $J_{cc}$. Both cell size and deformability were heterogeneous. Statistical significance was assessed by $t$ test (****: $p < 0.0001$).
Figure S6: (A) FACS gating strategy used for isolating mCSCs and hCSCs from MDA-MB-231 cells. Bar diagram shows percent positive mCSCs and hCSCs cells within MDA-MB-231 cells ($N = 6$). (B) Experimental setup for assaying percentage of nCSCs (CD44$^{-}\text{low}$), mCSCs and hCSCs within spheroids of MDA-MB-231 cells. (C) Bar diagram shows percent positive mCSCs and hCSCs cells within MDA-MB-231 spheroids ($n = 40, N = 2$). Statistical significance was determined by $t$ test ($**$: $p < 0.01; ***$: $p < 0.001$).
2. Supplementary Videos

Movie 1: Time lapse videos of random cell migration of MCF-7 and MDA-MB-231 cells over a duration of 24 hours with images acquired at 10 min intervals.

Movie 2: Representative videos of random scattering of homogeneous and heterogeneous cell clusters for three different values of $J_{CC} = 1$. 
Movie 3: Representative videos of random scattering of homogeneous and heterogeneous cell clusters for three different values of $J_{CC} = 16$.

Movie 4: Representative videos of random scattering of homogeneous and heterogeneous cell clusters for $J_{CC} = 40$. 
Movie 5: Video showing chemotaxis of a heterogeneous cluster for three different values of $J_{cc}$ for $\mu = 5000$.

Movie 6: Video showing chemotaxis of a heterogeneous cluster for three different values of $J_{cc}$ for $\mu = 2000$.

Movie 7: Video showing chemotaxis of populations comprising of (i) small cells of varying deformabilities (population A), (ii) soft cells of varying cell sizes (population B), and (iii) intermediately stiff cells of varying cell sizes (population C) for $J_{cc} = 1$ and $\mu = 5000$. 