Supporting material for

MemGen: A general web server for the setup of lipid membrane simulation systems

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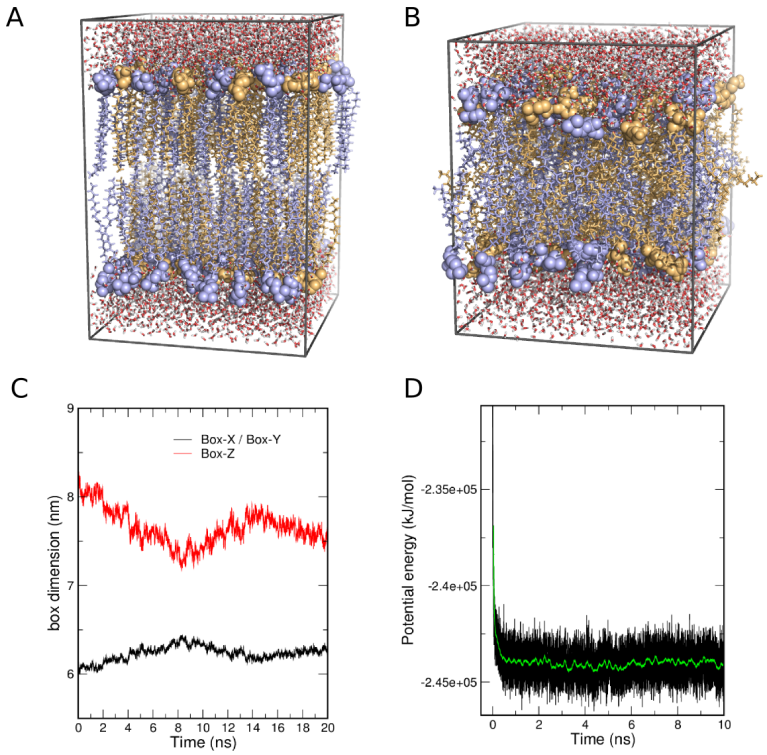

Figure S1. Equilibration of a simulation system containing 64 DOPC lipids, 64 DOPE lipids, and 4480 water molecules. Lipids are modelled by the SLipids force field. (A) MemGen output; (B) equilibrated patch after 5 ns; (C) equilibration of the box dimensions; (D) equilibration of the potential energy (black line). To guide the eye, a running average is shown in green (window width 100 ps).

Supporting discussion

Tested force fields

MemGen was so far tested with lipids from the following all-atom force fields: Charmm36 [Pastor and MacKerell Jr, 2011], SLipids [Jämbeck and Lyubartsev, 2012], GAFFlipid [Dickson *et al.*, 2012], Amber

lipids [Dickson *et al.*, 2014]. Memgen was tested with the following united-atom force fields: OPLS united-atom [Ulmschneider and Ulmschneider, 2009], Berger lipids [Berger *et al.*, 1997], Gromos-CKP [Piggot *et al.*, 2011], GROMOS53a6 [Kukol, 2009]. However, MemGen should work with any all-atom or united-atom representation of lipids.

Tested lipid types

MemGen was so far tested with at least the molecules in the following table.

Short name	Long name
DLPC	1,2-dilauroyl-sn-glycero-3-phosphocholine
DMPC	1,2-dimyristoyl-sn-glycero-3-phosphocholine
DPPC	1,2-dipalmitoyl-sn-glycero-3-phosphocholine
POPC	1-palmitoyl,2-oleoyl-sn-glycero-3-phosphocholine
DPPE	1,2-dipalmitoyl-sn-glycero-3-phosphoethanolamine
POPE	1-palmitoyl-2-oleoyl-sn-glycero-3-phosphoethanolamine
DOPS	1,2-dioleoyl-sn-glycero-3-phospho-L-serine
DPhyPC	1,2-diphytanoyl-sn-glycero-3-phosphocholine
DMPG	1,2-dimyristoyl-sn-glycero-3-phosphoglycerol
POPI	1-palmitoyl-2-oleoyl-sn-glycero-3-phosphoinositol
Lipid A	-
Cardiolipin	-
-	D-erythro-n-palmitoyl-sphingomyelin
PIP-2	1,2-dihexanoyl-sn-glycero-3-phospho-(1'-myo-inositol-3',5'-bisphosphate)
Cholesterol	-
Ergosterol	-
Progesterone	-
Progesterone sulfate	
DHEA	dehydroepiandrosteron
DHEA-S	dehydroepiandrosteron sulfate
1-octanol	-
1-decanol	-
BOG	n-octyl-beta-D-glucoside

Input parameters of MemGen

MemGen takes the following input parameters. Acceptable values are shown in brackets, and the default values in italic font:

- Lipids per monolayer (9–2500, *64*)
- Water molecules per lipid (0-100, *35*)
- Salt concentration (mMolar) (0-10.000, *0*)
- Area per lipid ($Å^2$) (20-100, *65*).

References

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