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User Manual by Elmar.Krieger@yasara.org Date of last revision: 2012/01/06 NOTE: Models@Home has been developed in 2000 at the CMBI/Radboud University Nijmegen, and has since been used for all computationally intensive tasks at YASARA.org, like force field parameter optimization or large scale homology modeling.

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Select the appropriate combination of operating systems such that the master's OS is listed first. Then copy the updated YASARA folder to your other machines. 2) Update each installation independently. In this case, always type in the YASARA version you want to update and choose the right operating system and processor.

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YASARA - Products

YASARA runs for each block the md_analyze macro and creates in the end a single report containing detailed information about the system, e.g. energies, RMSDs, hydrogen bonds per block. By default the simulation snapshots are split into 3 blocks, so the second and third block can be compared to see if convergence has been reached.

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Chapter 2 The YASARA user interface | A Guide to YASARA

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Installation and first use - FoldX plugin for YASARA

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