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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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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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