VANDERBILT UNIVERSITY

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Homework 07

- is to be submitted for grading after 1 week in class; no late submissions are accepted
- show your work neatly – if I do not understand logic in your steps, you will lose points
- make a sincere effort to understand the problems; otherwise you may not do well on the presentation and on the exams

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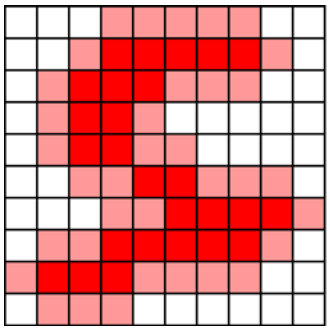
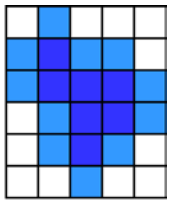
1. Dock the blue shape into red shape testing translational and rotational (0°,90°,180°,270°) degrees of freedom. Dark color represents the interior with a base value of $b_{int} = -10$, light color the surface with a base value of $b_{surf} = 2$, and white the solvent with a base value of $b_{surf} = 0$. The total score is computed as sum $S = \sum_{ij} b_i^{blue} \times b_j^{red}$ over all overlapping squares. Report best three docking poses with scores!





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