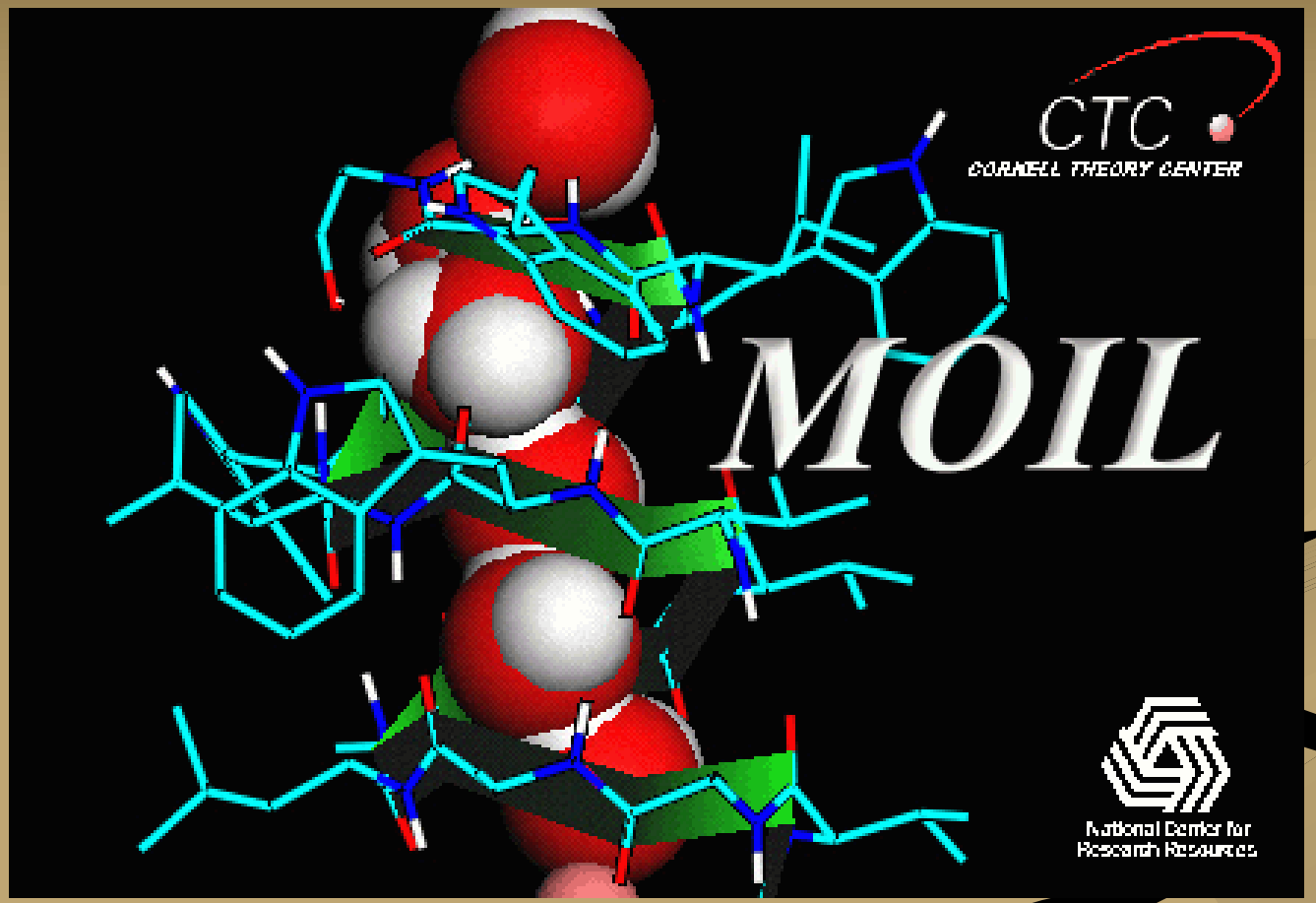
CTC
CORNELL THEORY CENTER
MOIL
National Center for
Research Resources

# What is MOIL?

- A suite of programs to study proteins, other biologically macromolecules and liquids
- Programs are written in FORTRAN and the source code is available for free at http://cbsu.tc.cornell.edu/software/proteins_dynamics.htm

# What MOIL can do for you?

# Processing PDB files for further molecular simulations or visualization

```
HETATM    1  C   FOR A   1A     -3.690  -1.575  -2.801  1.00  0.00           C
HETATM    2  O   FOR A   1A     -3.774  -1.363  -1.586  1.00  0.00           O
HETATM    3  H   FOR A   1A     -4.305  -1.047  -3.545  1.00  0.00           H
ATOM      4  N   VAL A   1      -3.043  -2.601  -3.416  1.00  0.00           N
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ATOM      7  O   VAL A   1      -0.385  -3.961  -3.851  1.00  0.00           O
ATOM      8  CB  VAL A   1      -2.919  -5.045  -2.884  1.00  0.00           C
ATOM      9  CG1 VAL A   1      -2.163  -6.141  -2.056  1.00  0.00           C
ATOM     10  CG2 VAL A   1      -4.427  -5.132  -2.644  1.00  0.00           C
ATOM     11  H   VAL A   1      -2.760  -2.649  -4.381  1.00  0.00           H
ATOM     12  HA  VAL A   1      -2.651  -3.401  -1.570  1.00  0.00           H
ATOM     13  HB  VAL A   1      -2.542  -5.494  -3.836  1.00  0.00           H
ATOM     14 1HG1 VAL A   1      -2.280  -5.946  -0.974  1.00  0.00           H
ATOM     15 2HG1 VAL A   1      -2.578  -7.146  -2.278  1.00  0.00           H
ATOM     16 3HG1 VAL A   1      -1.080  -6.174  -2.292  1.00  0.00           H
ATOM     17 1HG2 VAL A   1      -4.671  -4.794  -1.613  1.00  0.00           H
ATOM     18 2HG2 VAL A   1      -4.985  -4.505  -3.373  1.00  0.00           H
ATOM     19 3HG2 VAL A   1      -4.766  -6.182  -2.771  1.00  0.00           H
ATOM     20  N   GLY A   2      -0.150  -3.167  -1.782  1.00  0.00           N
ATOM     21  CA  GLY A   2       1.289  -3.155  -2.035  1.00  0.00           C
ATOM     22  C   GLY A   2       2.025  -2.270  -1.112  1.00  0.00           C
ATOM     23  O   GLY A   2       1.812  -2.330   0.088  1.00  0.00           O
ATOM     24  H   GLY A   2      -0.506  -2.978  -0.859  1.00  0.00           H
ATOM     25 1HA  GLY A   2       1.662  -4.152  -1.871  1.00  0.00           H
ATOM     26 2HA  GLY A   2       1.469  -2.805  -3.044  1.00  0.00           H
ATOM     27  N   ALA A   3       2.946  -1.447  -1.648  1.00  0.00           N
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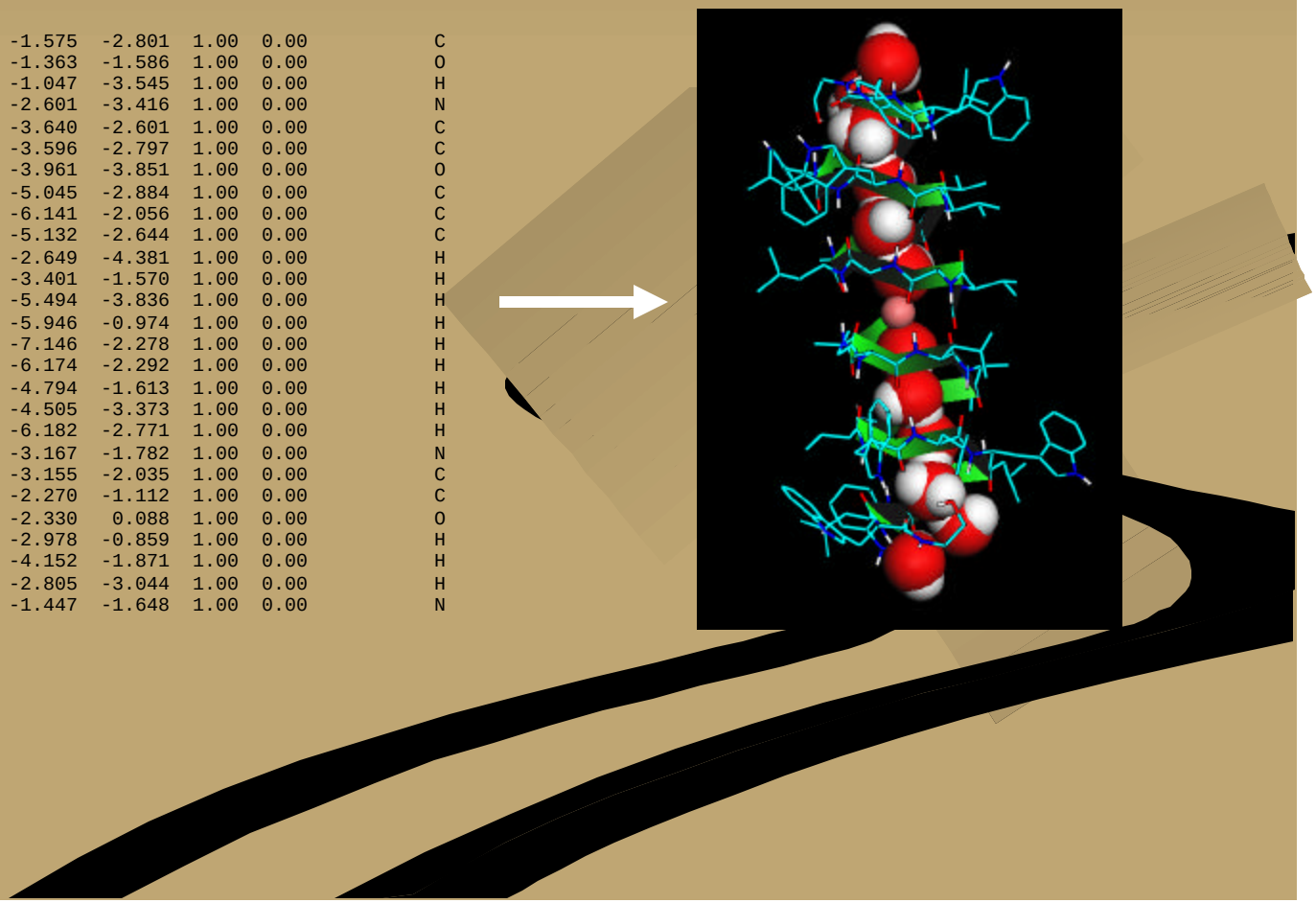
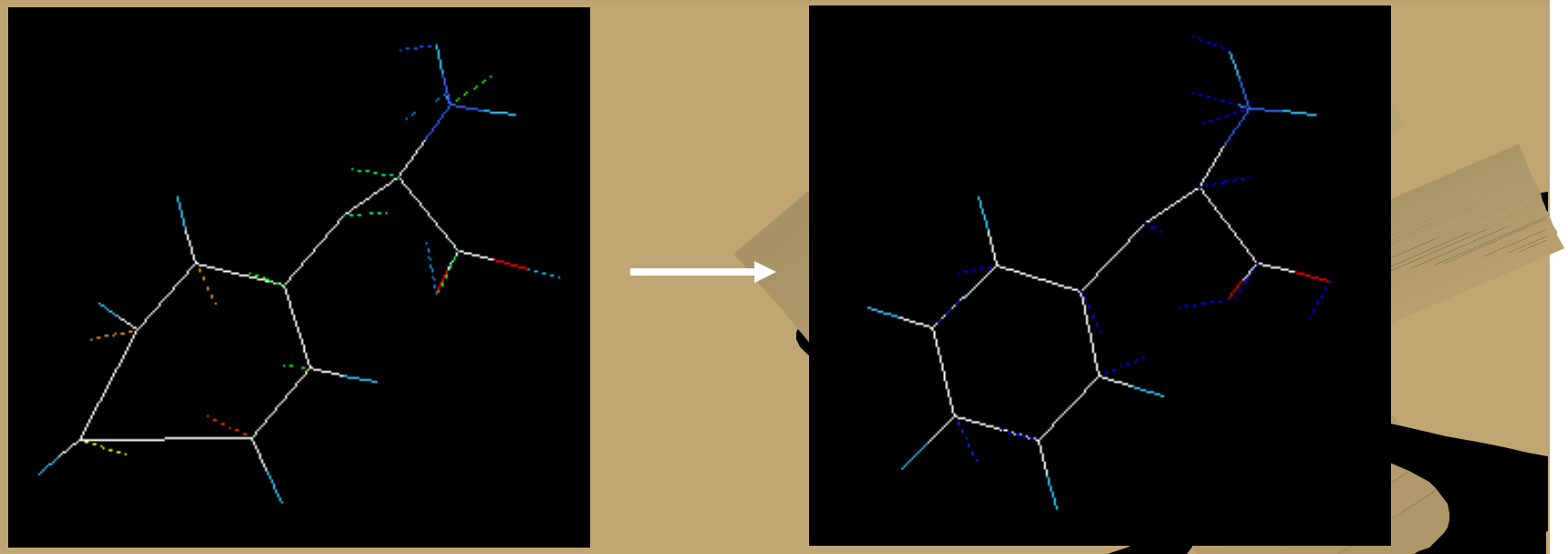
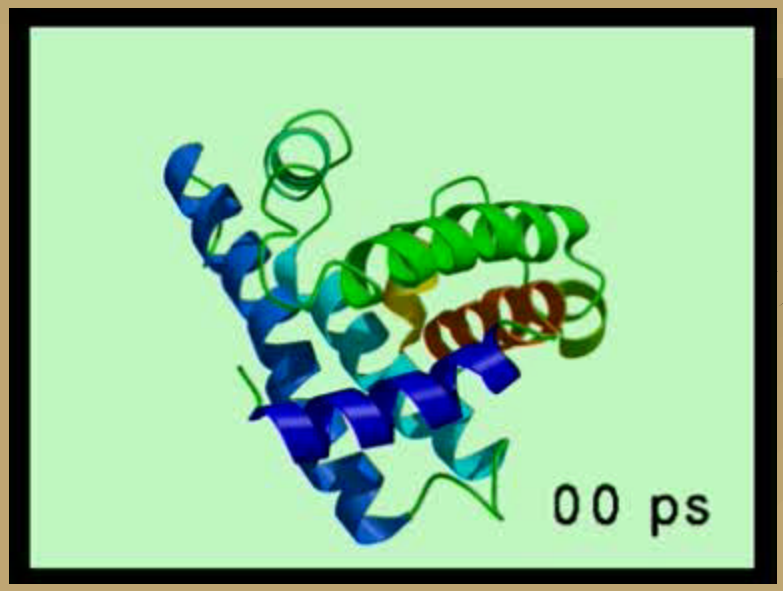


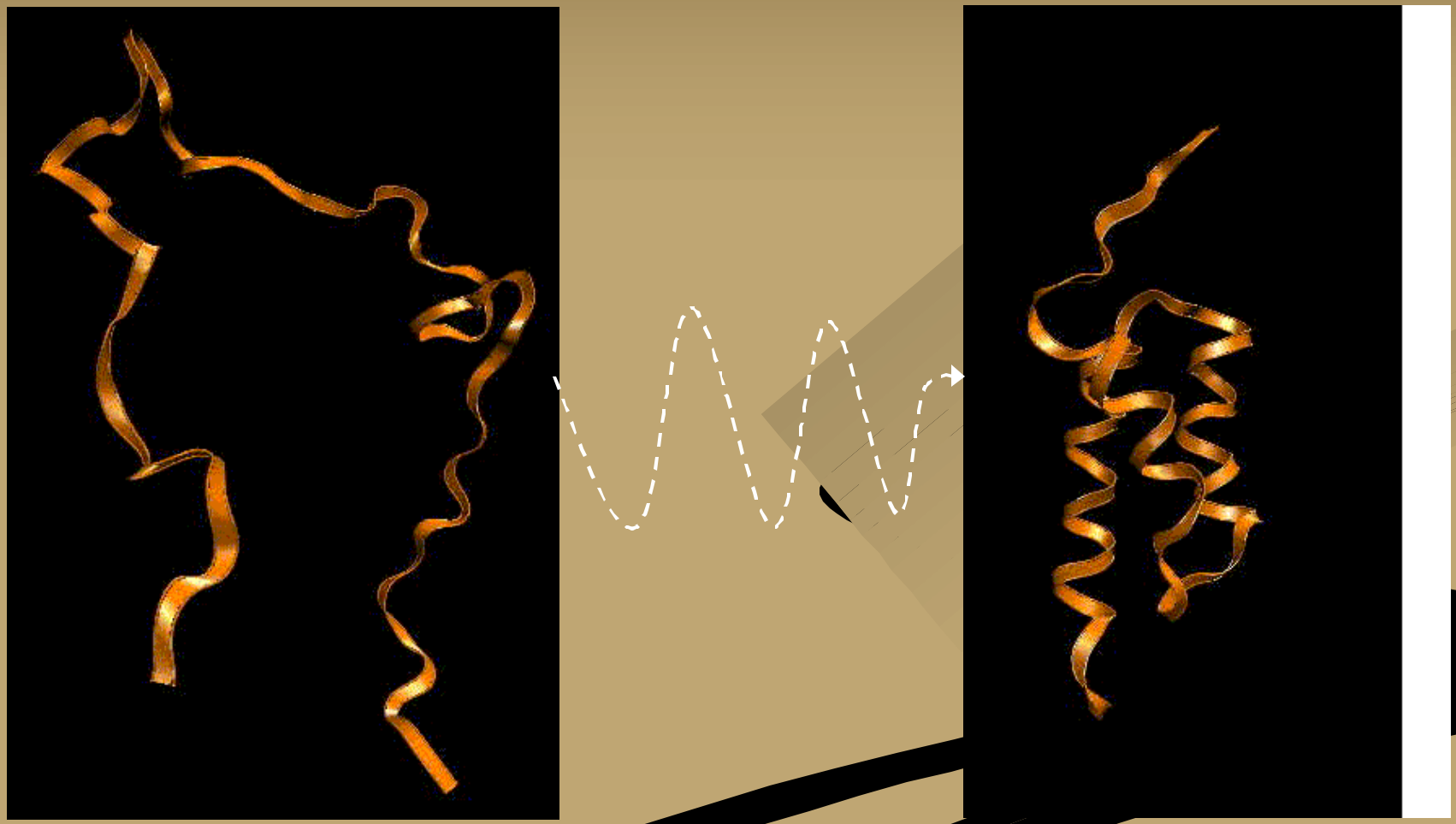
# Molecular energy calculations
# Molecular energy minimizations



# Conventional Molecular Dynamics



# Path energy minimization
# Path-based long-time MD

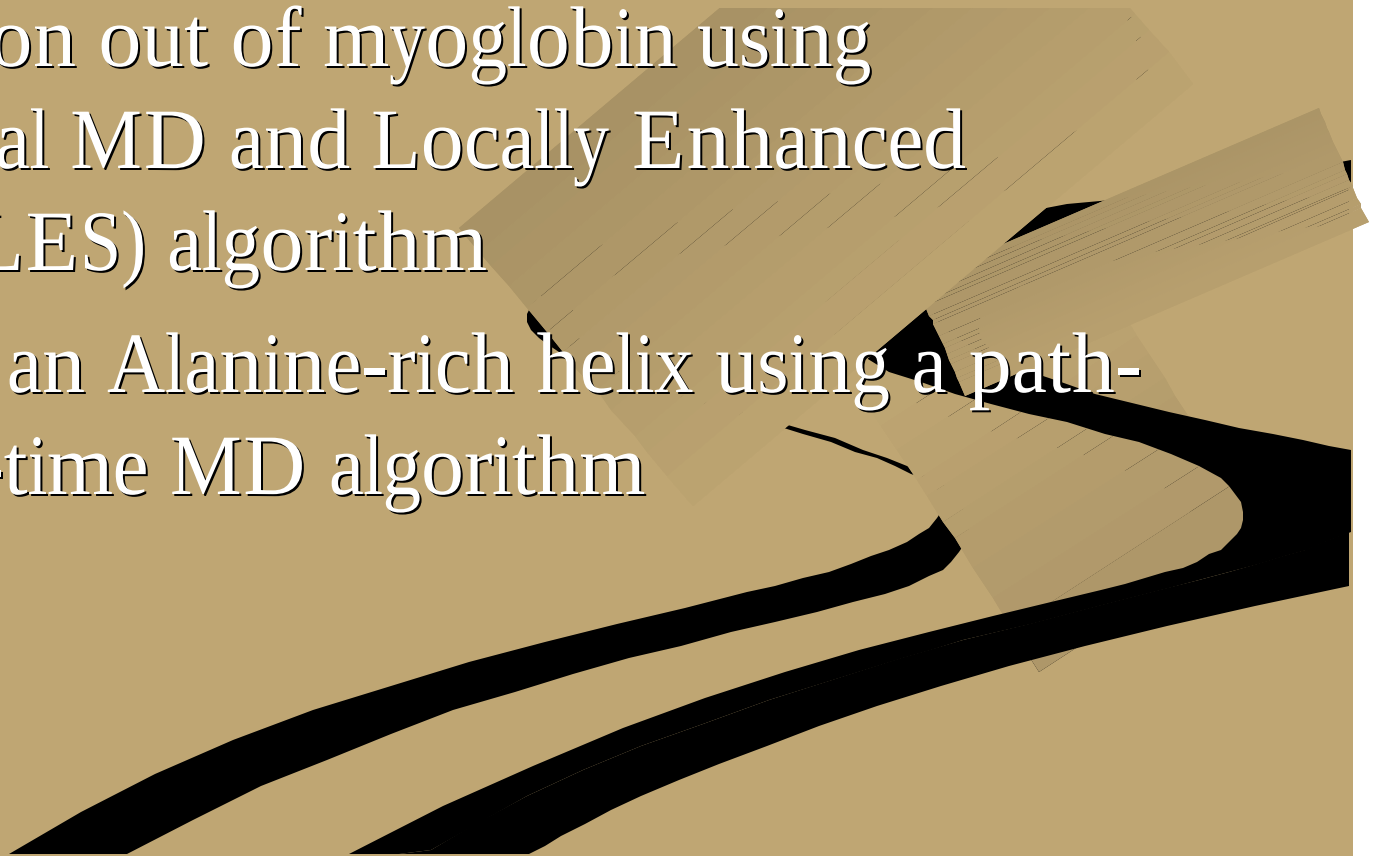


# Subdirectories in MOIL

- Moil.mop
  - AMBER/OPLS force field files: ALL.MONO and ALL.PROP
  - All-atom AMBER force field files: PROTEIN.MONO and AMBER.PROP
- Moil.doc
  - Documentation and tutorials
- Moil.test9
  - Runs examples with their corresponding input and output files
- Moil.source

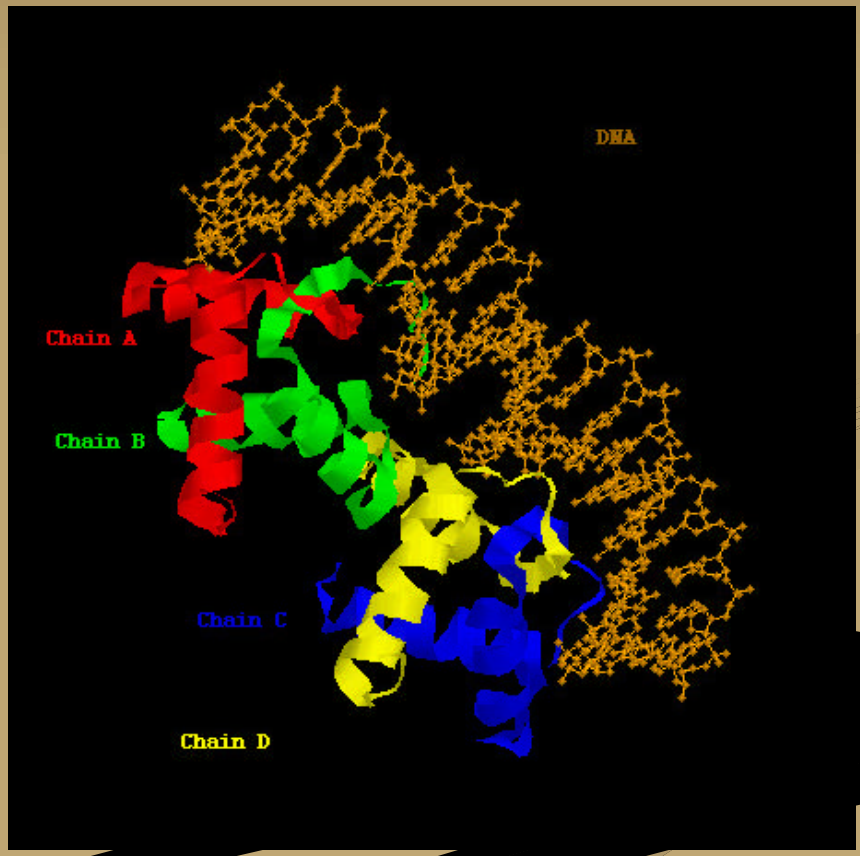
# Examples

1) Solvation and visualization of the Arc Repressor protein dimer from its PDB file
2) CO diffusion out of myoglobin using conventional MD and Locally Enhanced Sampling (LES) algorithm
3) Folding of an Alanine-rich helix using a path-based long-time MD algorithm



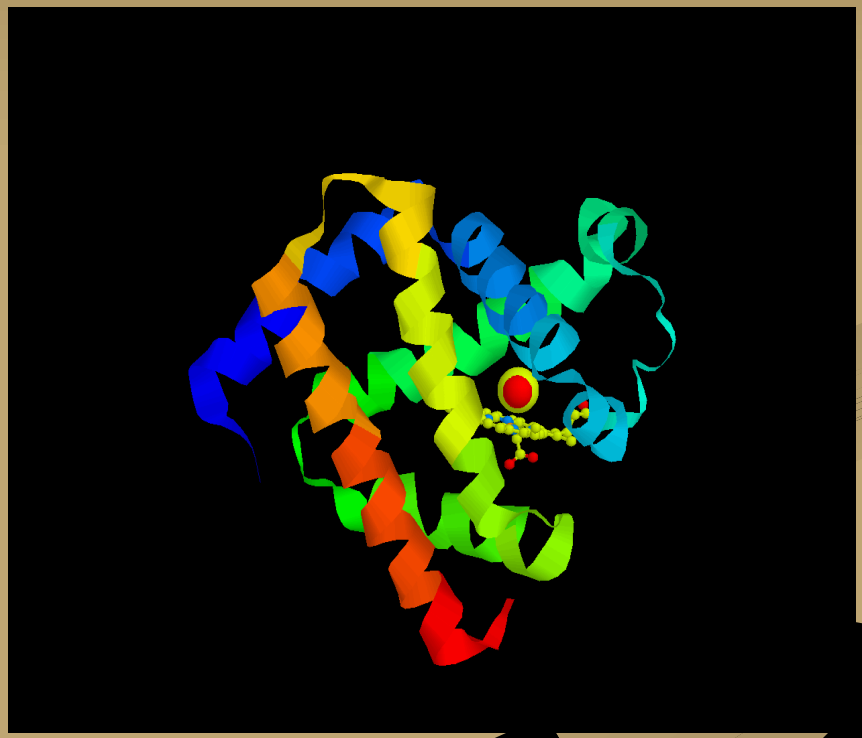
# Solvation of Arc Repressor

- Use MOIL to read pdb file and obtain sequence information (poly file), connectivity information (wcon file) and convert from pdb -> crd file
- Solvation of the protein in a box of water molecules
- Visualization tools



# CO diffusion out of myoglobin

- Create a connectivity file (wcon) from a sequence (poly) file
- Use of LES to enhance the observation in a part of the molecule
- Energy minimization
- Molecular Dynamics
- Analysis tools



# Folding dynamics of an Alanine-rich helix

- Use of Path energy minimization to obtain a guess for the MD path between unfolded and folded structures
- Use of a path-based long time MD algorithm to compute the helix-coil kinetics