Study Of Protein Folding

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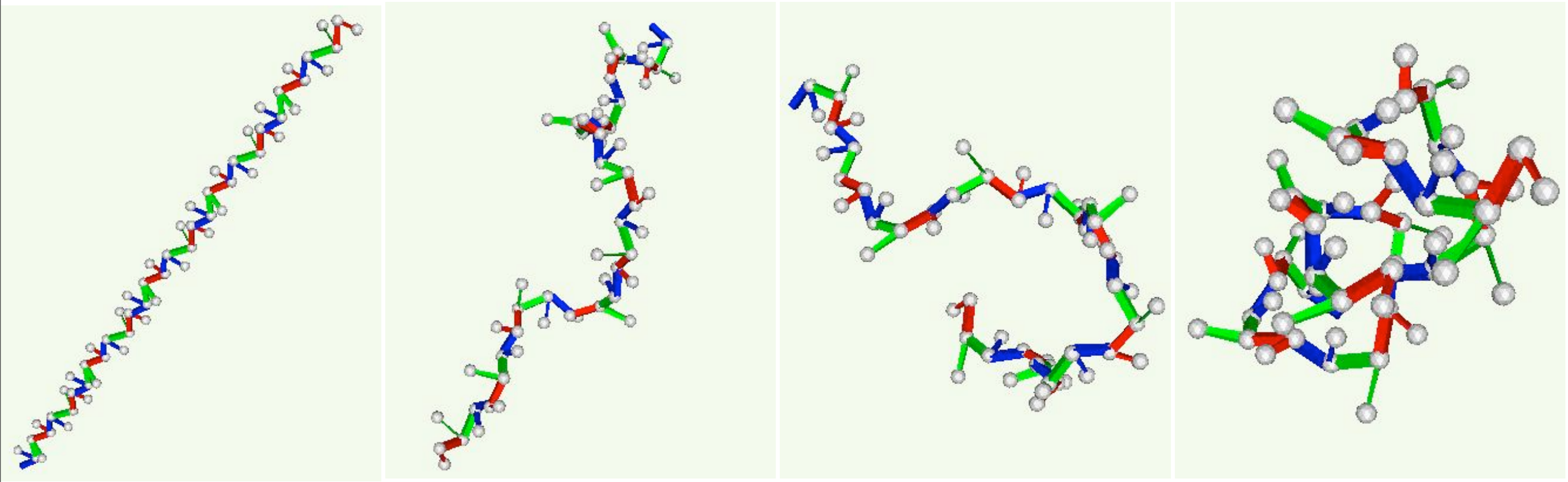
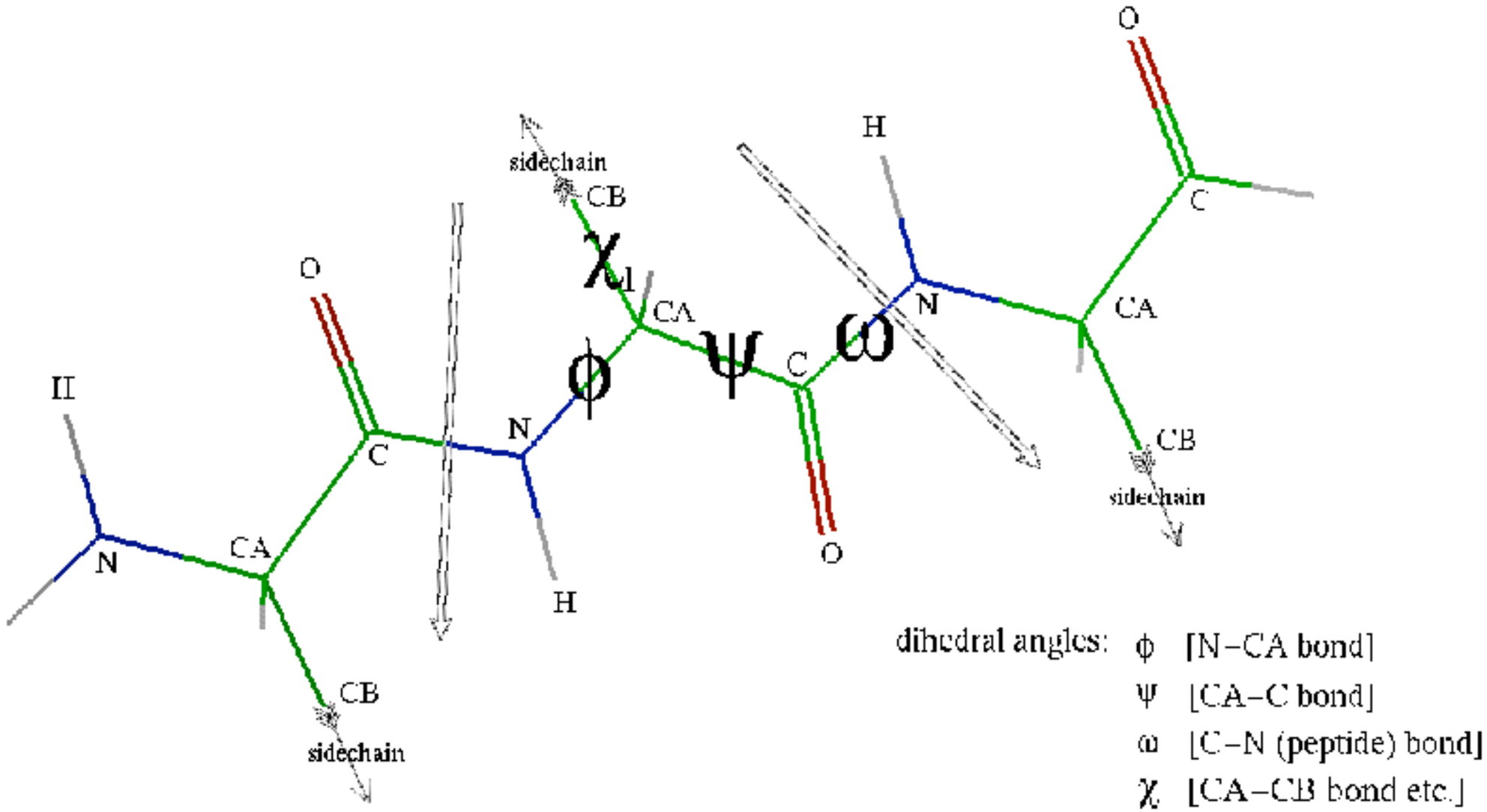
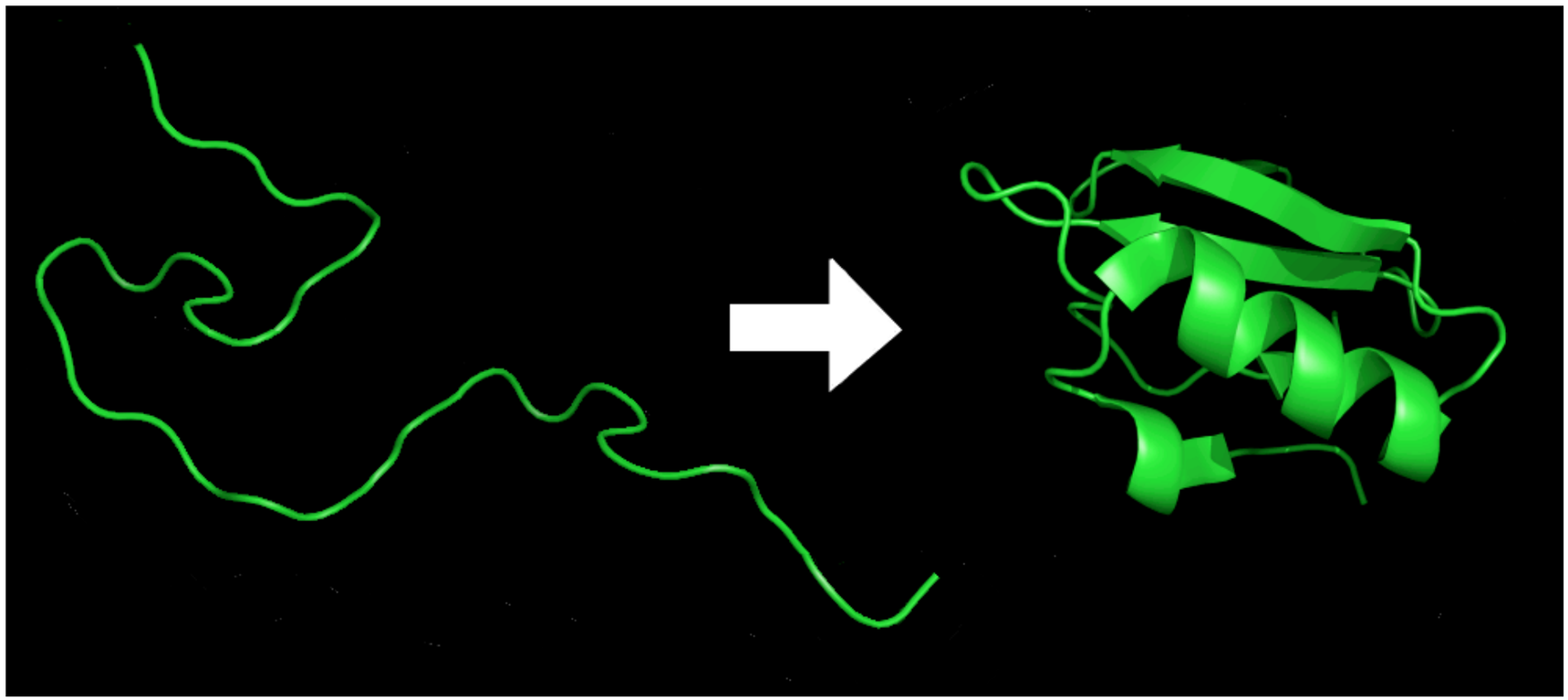


Folding snapshots of a 10-ALA chain [1]



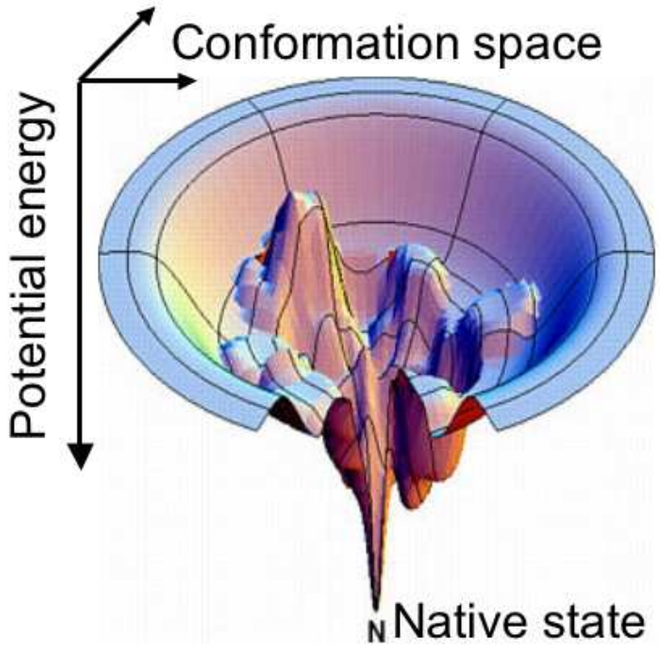
Amino acid model; each amino acid has 2 degrees of freedom, the phi and psi torsional angles. [2]

Levinthal's Paradox

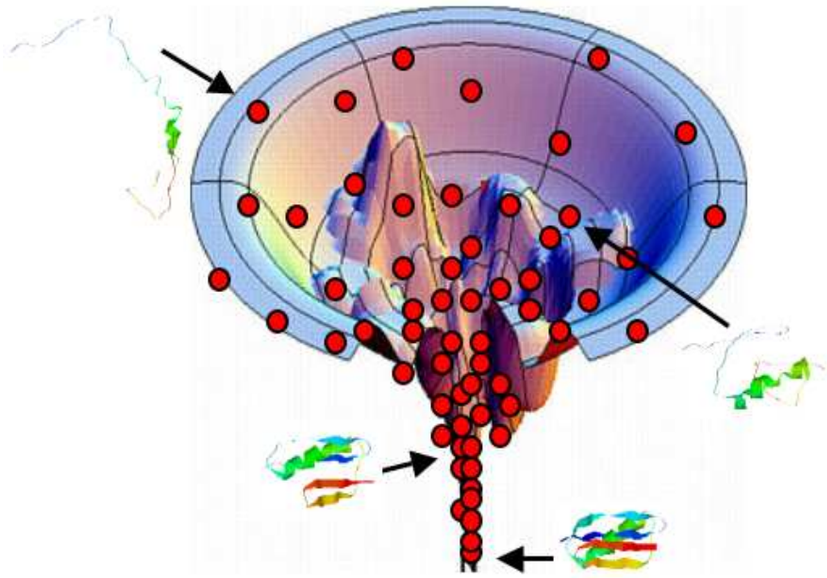


[3]

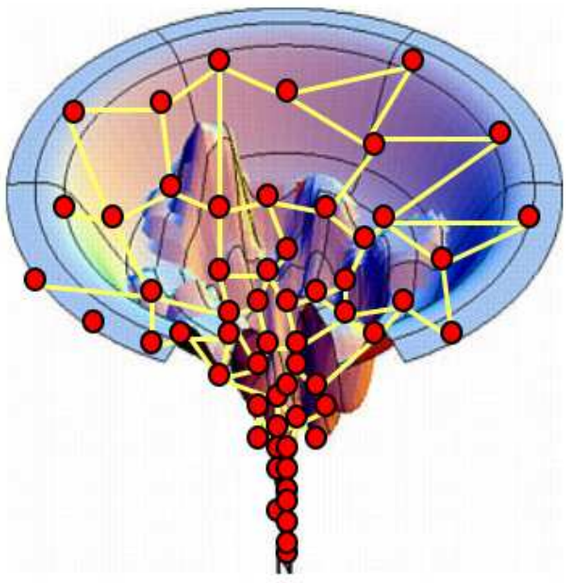
NP or P ?



Potential Energy Landscape



Conformation Sampling



Feasible Transitions

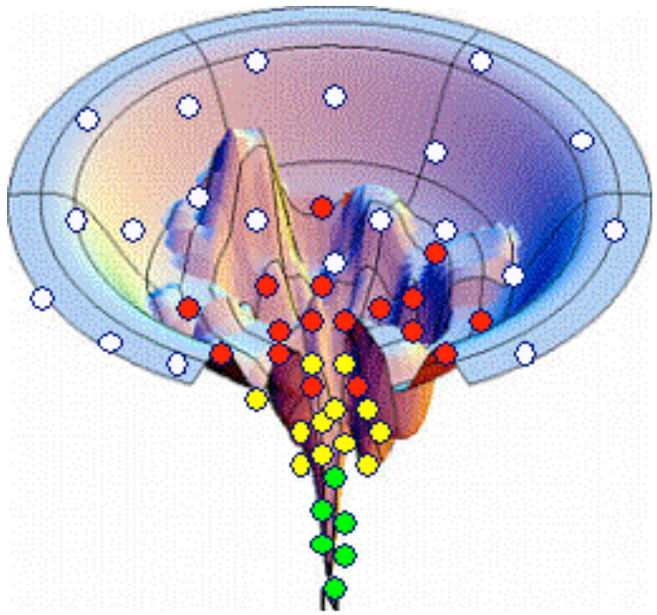
[4]

$$U_{tot} = \sum_{restraints} K_d\{[(d_i - d_0)^2 + d_c^2]^{1/2} - d_c\} + E_{hp}$$

$$Prob(\text{accept q}) = \begin{cases} 1 & \text{if } E_q < E_{\min} \\ \frac{E_{\max} - E_q}{E_{\max} - E_{\min}} & \text{if } E_{\min} \leq E_q \leq E_{\max} \\ 0 & \text{if } E_q > E_{\max} \end{cases}$$

$$P_i = \begin{cases} e^{\frac{-\Delta E_i}{kT}} & \text{if } \Delta E_i > 0 \\ 1 & \text{if } \Delta E_i \leq 0 \end{cases}$$

Sampling Strategy



[5]

Bins filled according to the Contact Number of a conformation

Code and Data Available

- Data Available in PDB files [Protein Data Bank]
- Code available for calculating Dihedral Angles(Phi, Psi) from Coordinates of atom.[google code library]

Code we have Written

- To calculate energy of a conformation from the atom coordinates.
- For generating sample nodes by using inducing Gaussian perturbations in existing conformations.
- To calculate atom coordinates from the dihedral angles of a node sampled.

References

- [1] An Motion Planning Approach to Folding: From Paper Crafts to Protein Folding.
  supported by NSF
  Guang Song, Nancy Amato, Ken Dill (UCSF), Lawrence Rauchwerger

- [2] parasol.tamu.edu

- [3] wikipedia.org

- [4] A MOTION PLANNING APPROACH TO STUDYING MOLECULAR MOTIONS∗LYDIA TAPIA†, SHAWNA THOMAS†, AND NANCY M. AMATO†

- [5] parasol.tamu.edu