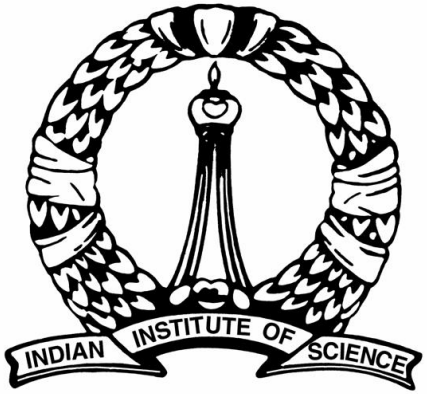
Improved Quadric Surface Impostors for Large Bio-Molecular Visualization



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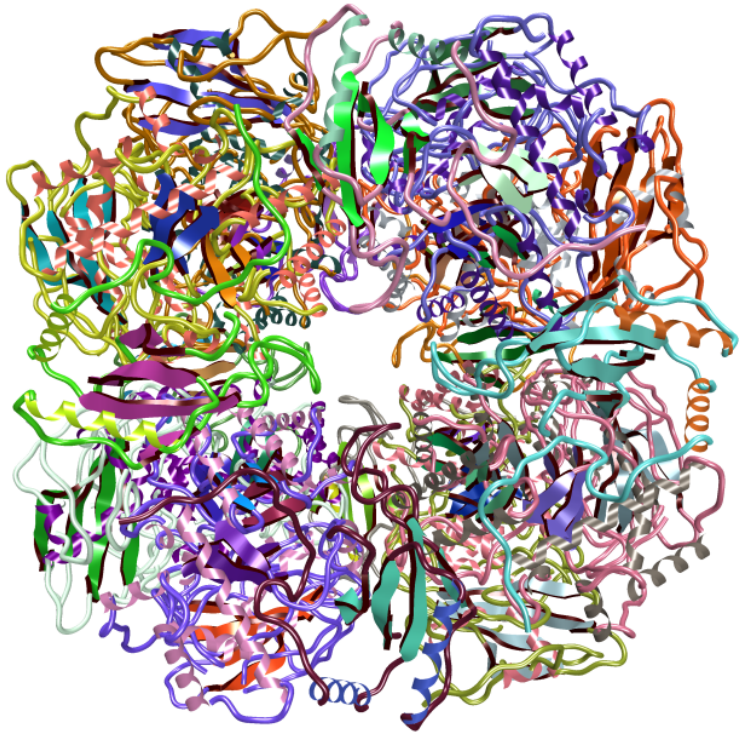
Motivation

The Need for Bio-Visualization

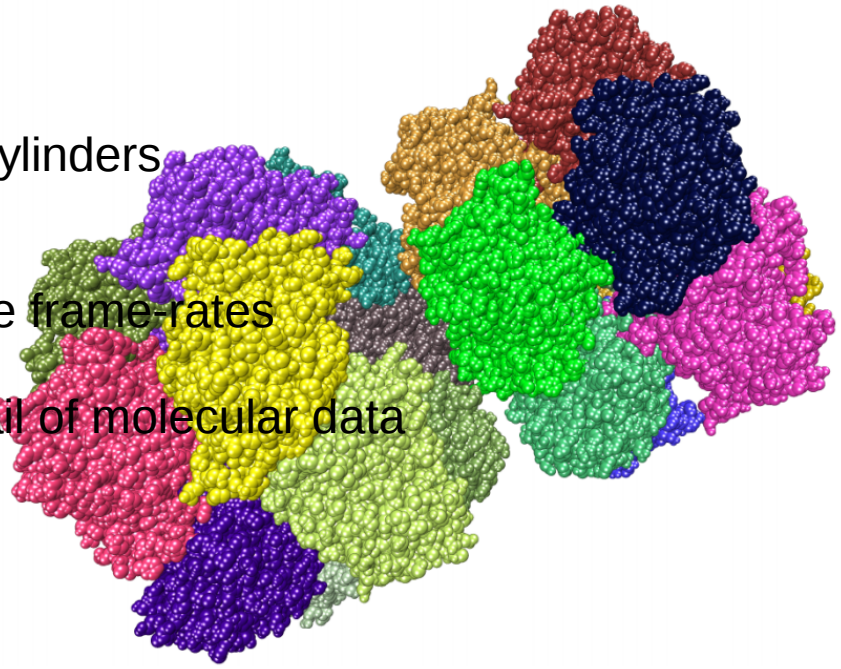
- To better understand the overall structure of proteins
- Insight into protein folding



s, cylinders

ctive frame-rates

detail of molecular data

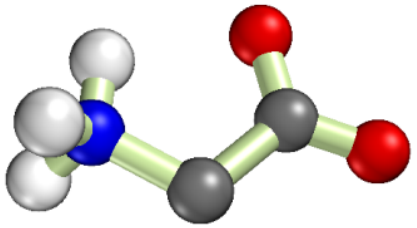


Contributions

The Unified Two Step Framework

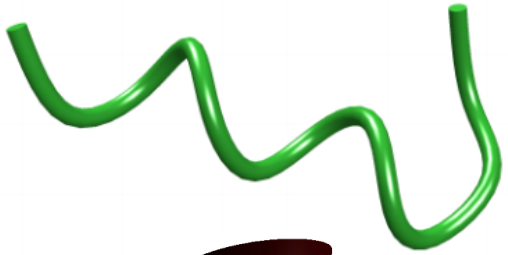
Spherical Elements

- Simplified ellipsoid model
- [Gumhold, VMV 2003]



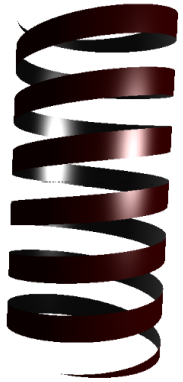
Cylindrical Elements

- Non-Parallel caps
- Extension to tubes

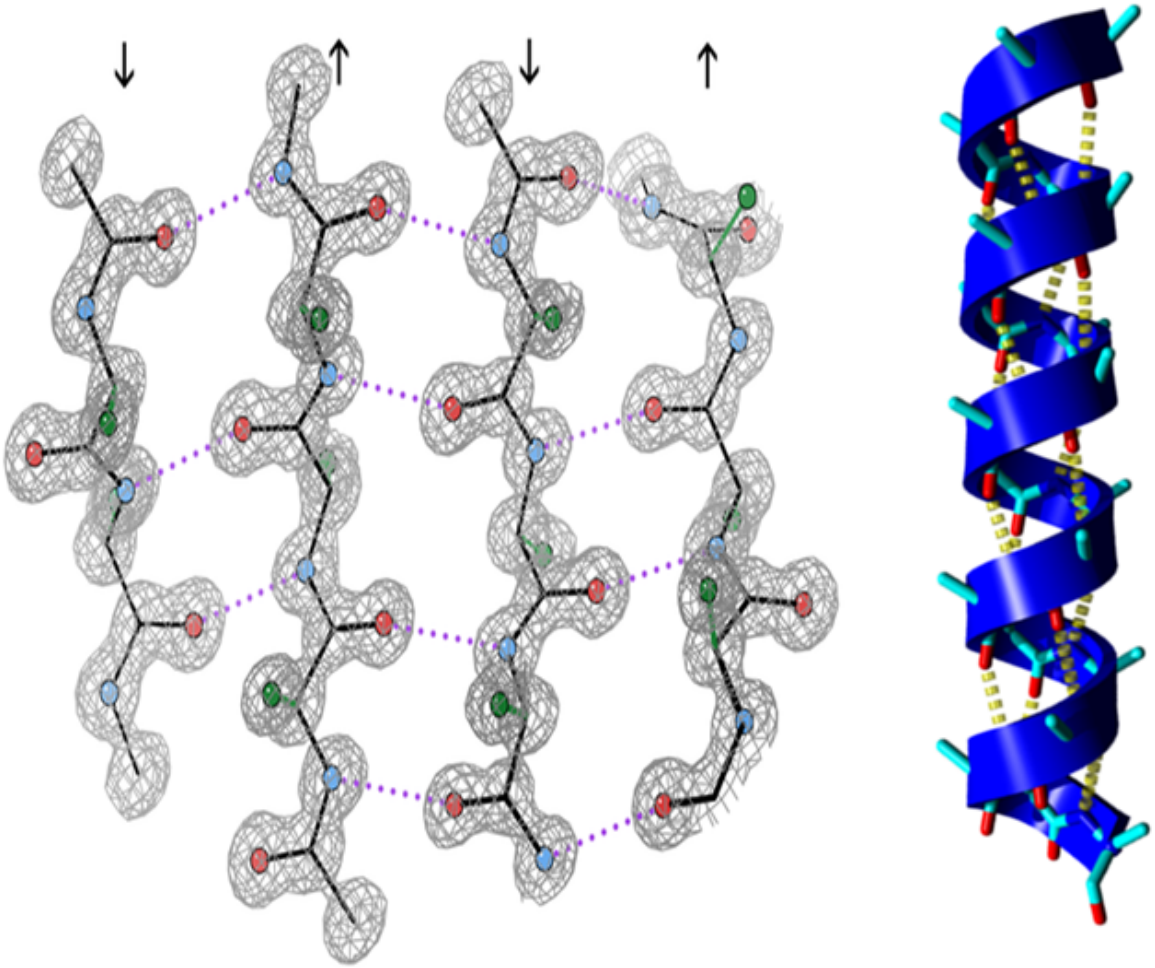


Helical Elements

- Extension of Cylindrical Impostors

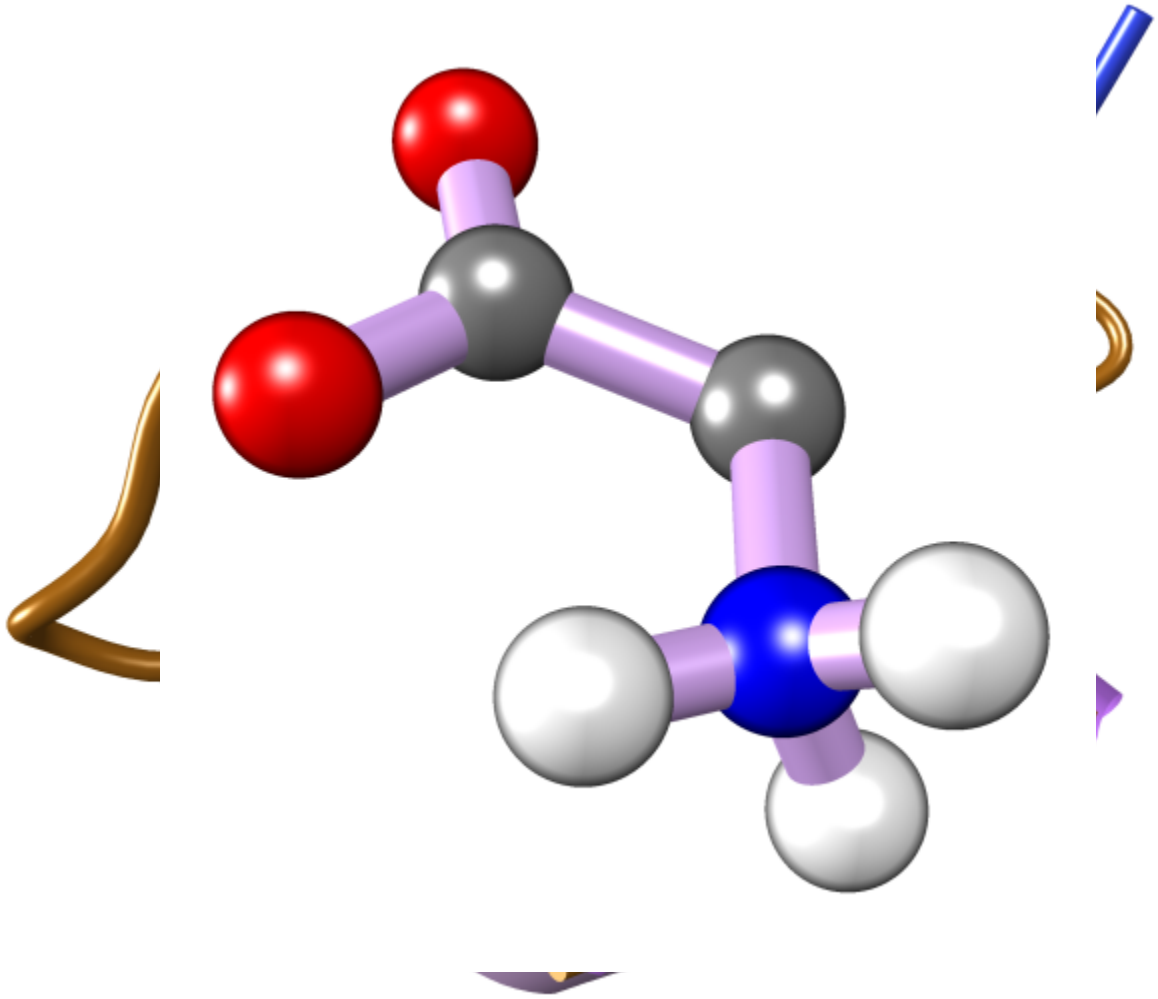


Background



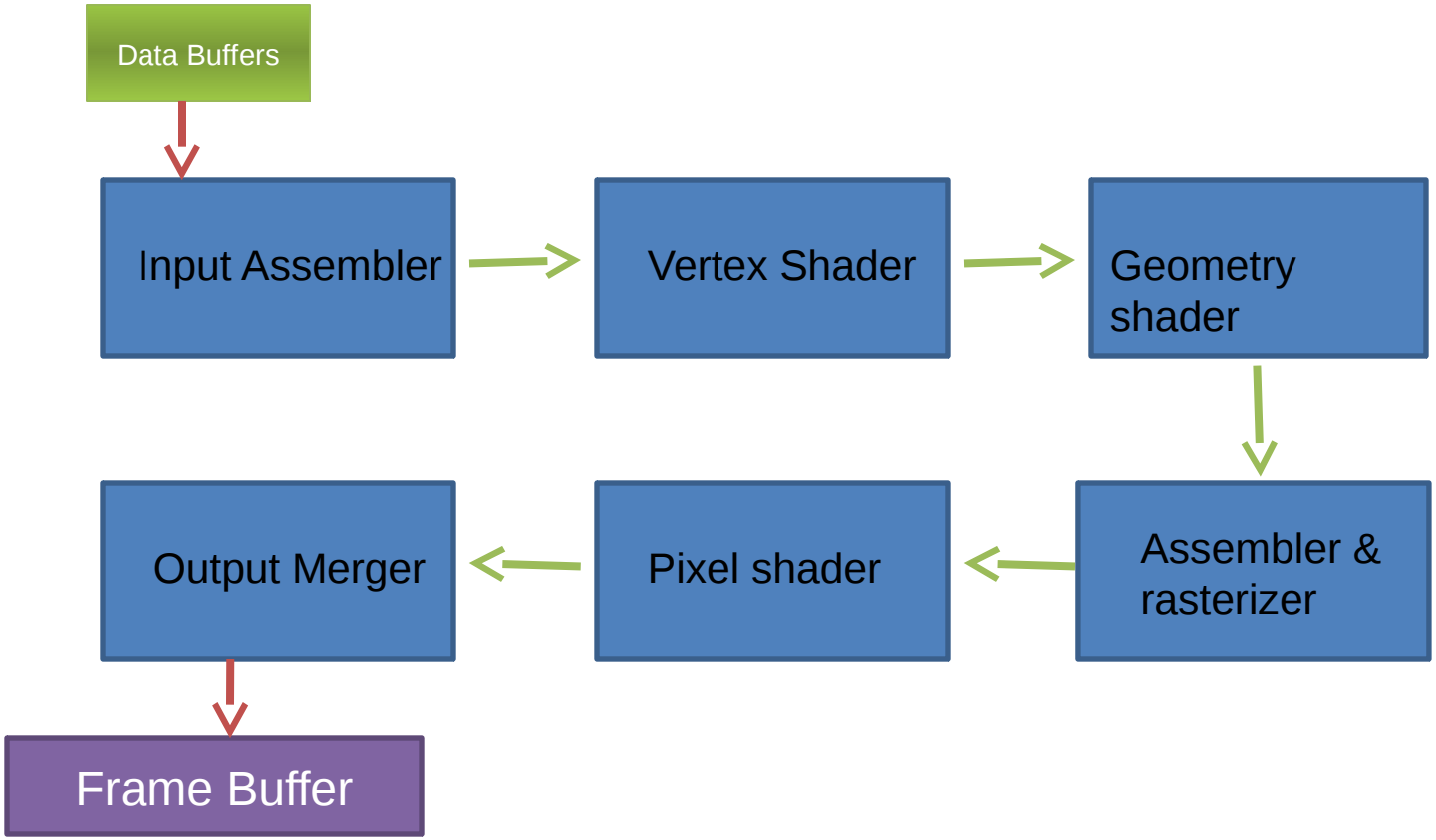
Proteins

- A linear polymer chain of amino acids bonded together by peptide bonds.
- Proteins usually coil into α-helices, β-sheets or random coils.



Protein Visualization

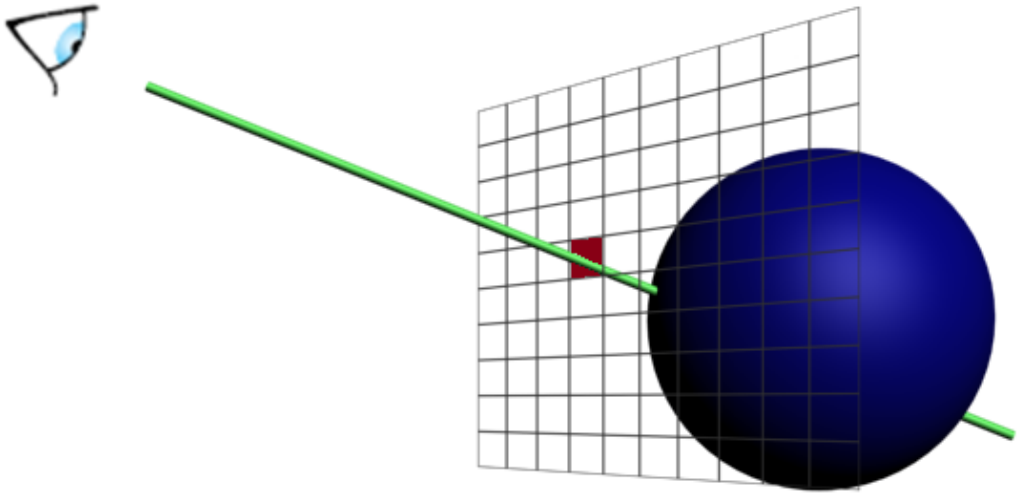
- Space fill model visualizes the atoms with spheres
- Ball-stick model explicitly shows the bonding with cylinders.
- The secondary structure models the protein folding.



Graphics pipeline

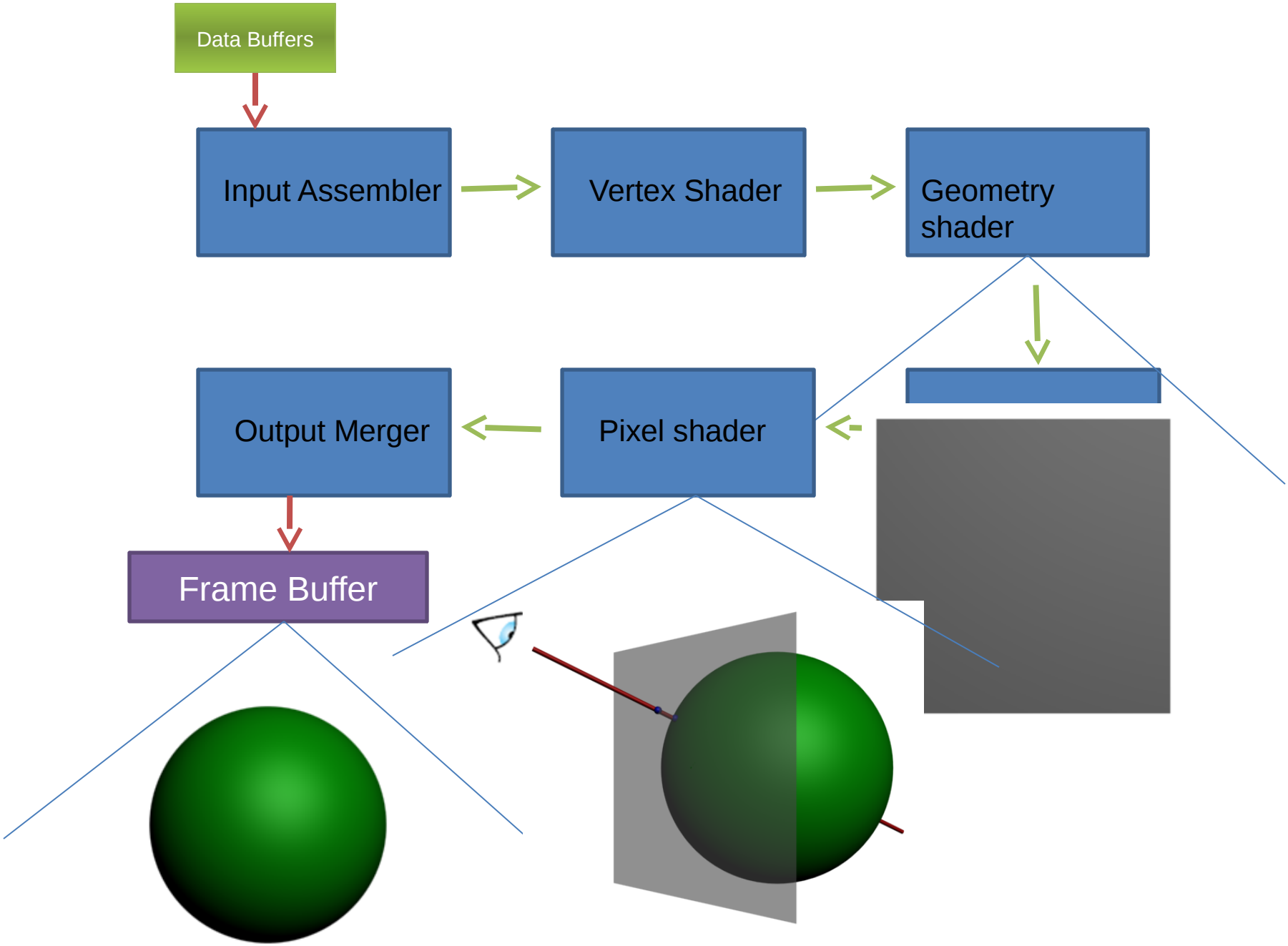
- Transforms primitives in 3-D space to pixels on screen
- Some parts of the pipeline are programmable

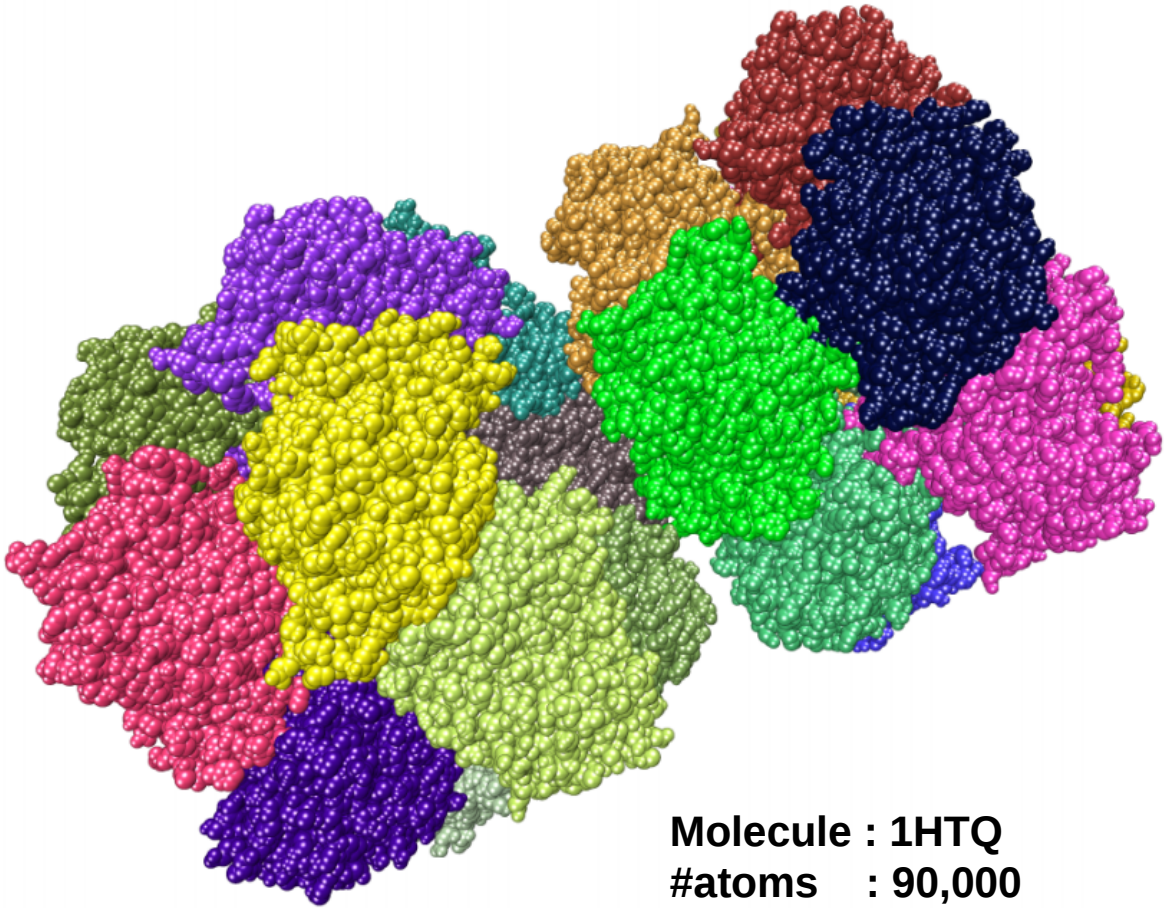
Impostoring and Its Applications



Two-step Impostor framework

- Primary stage produces Impostor primitives
- Secondary stage puts these elements together

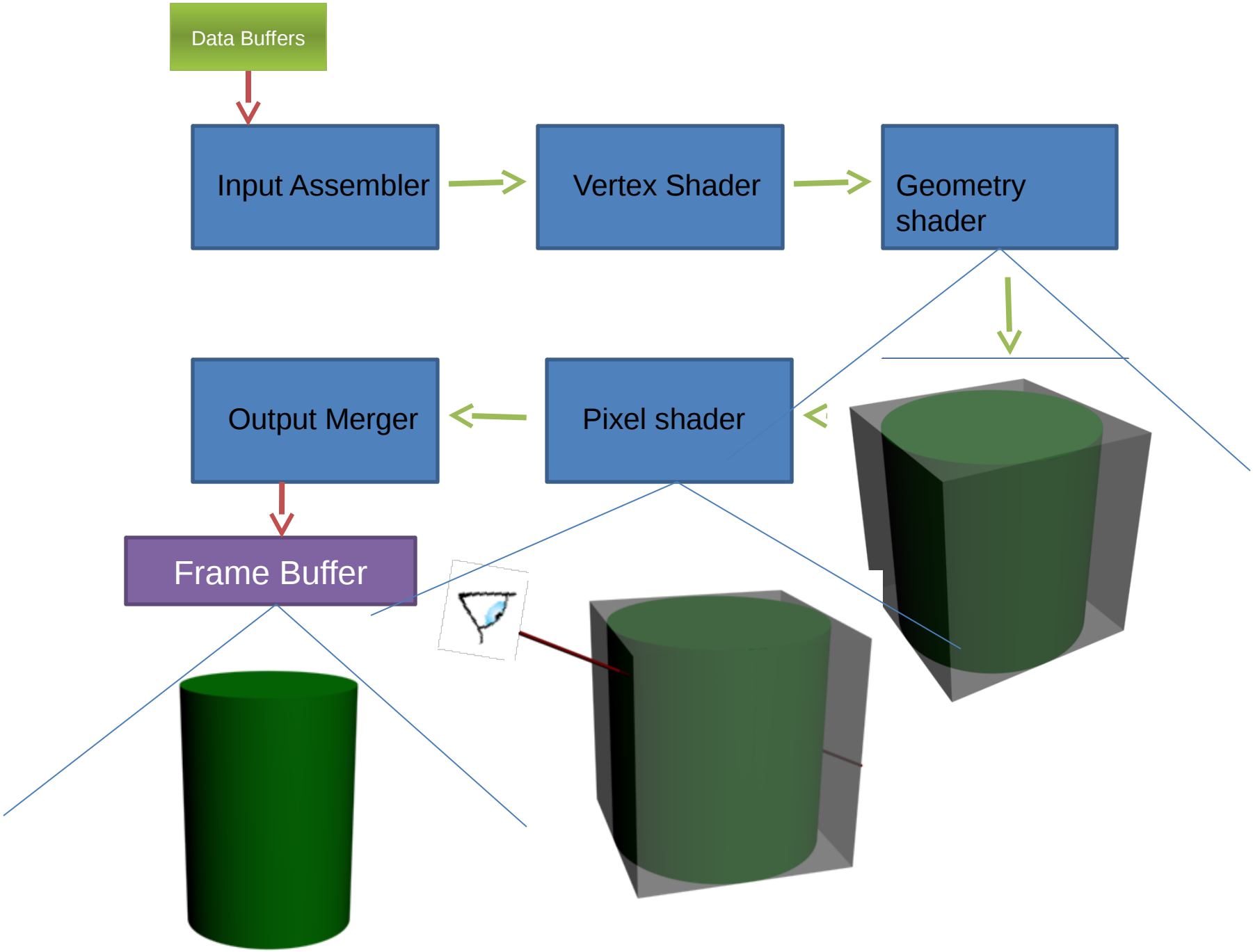

Data Buffers
Input Assembler
Vertex Shader
Geometry shader
Output Merger
Pixel shader
Frame Buffer



Molecule : 1HTQ
#atoms : 90,000

Space-fill using spherical Impostors

- Atomic centers are replaced by spheres with van-der Waals radius
- Colored according to chains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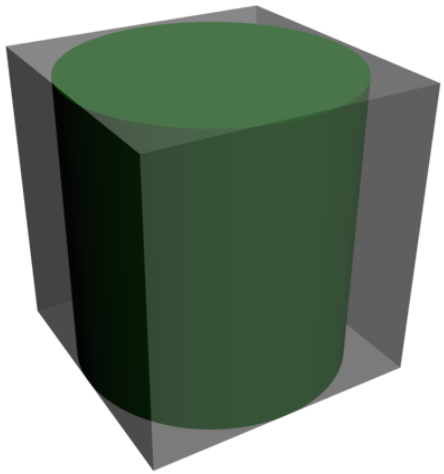
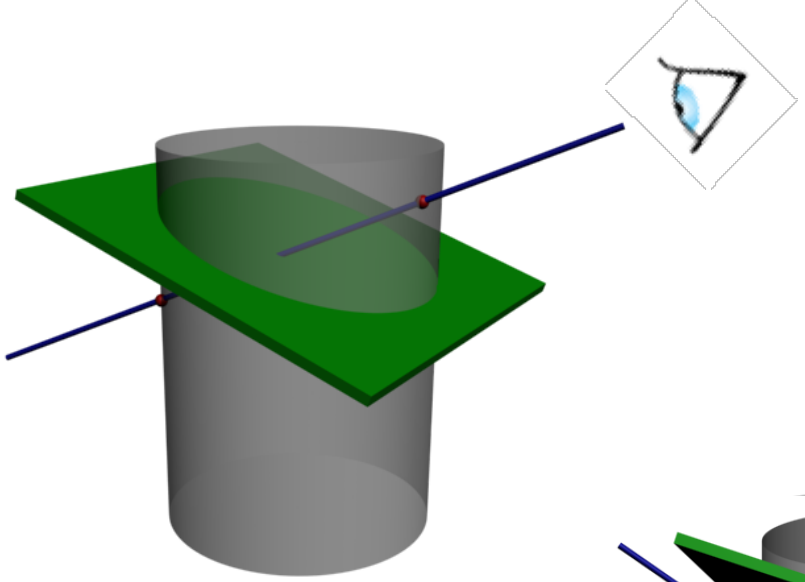
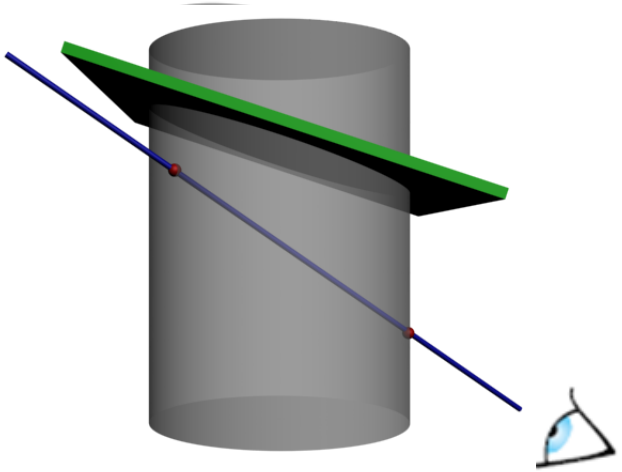
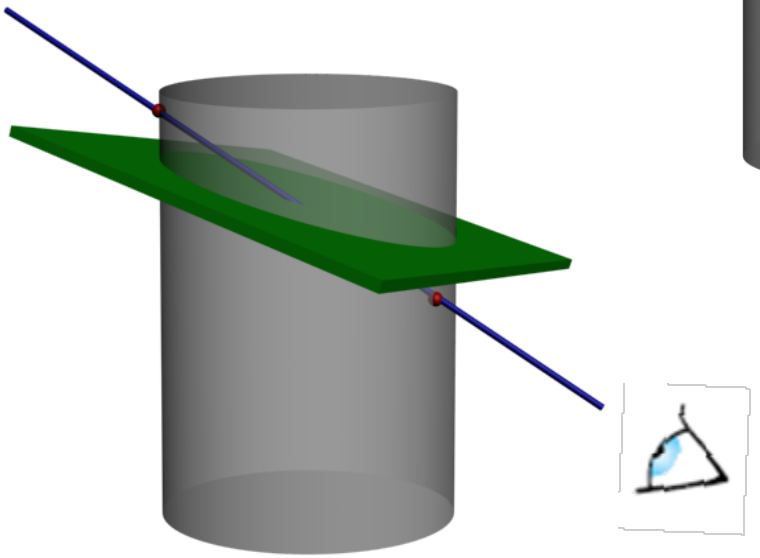




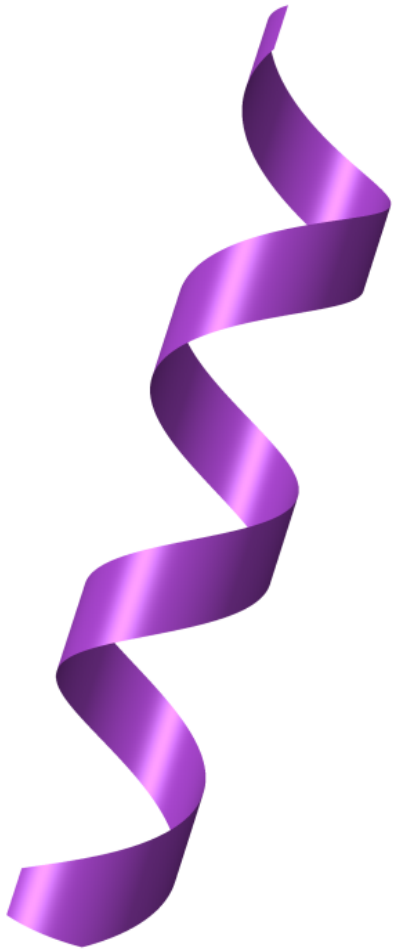




[Krone et.al]

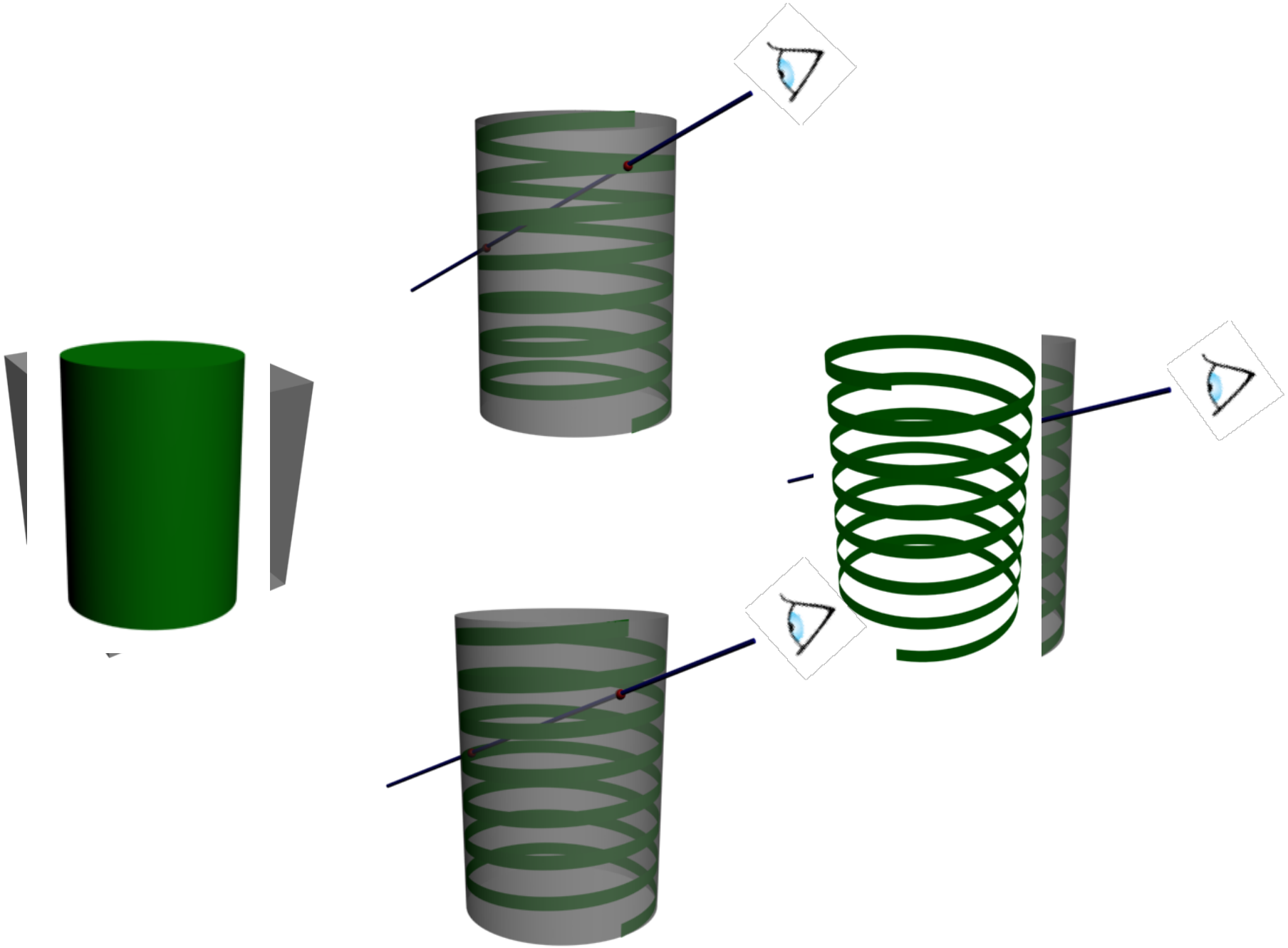
Tubes using cylindrical Impostors

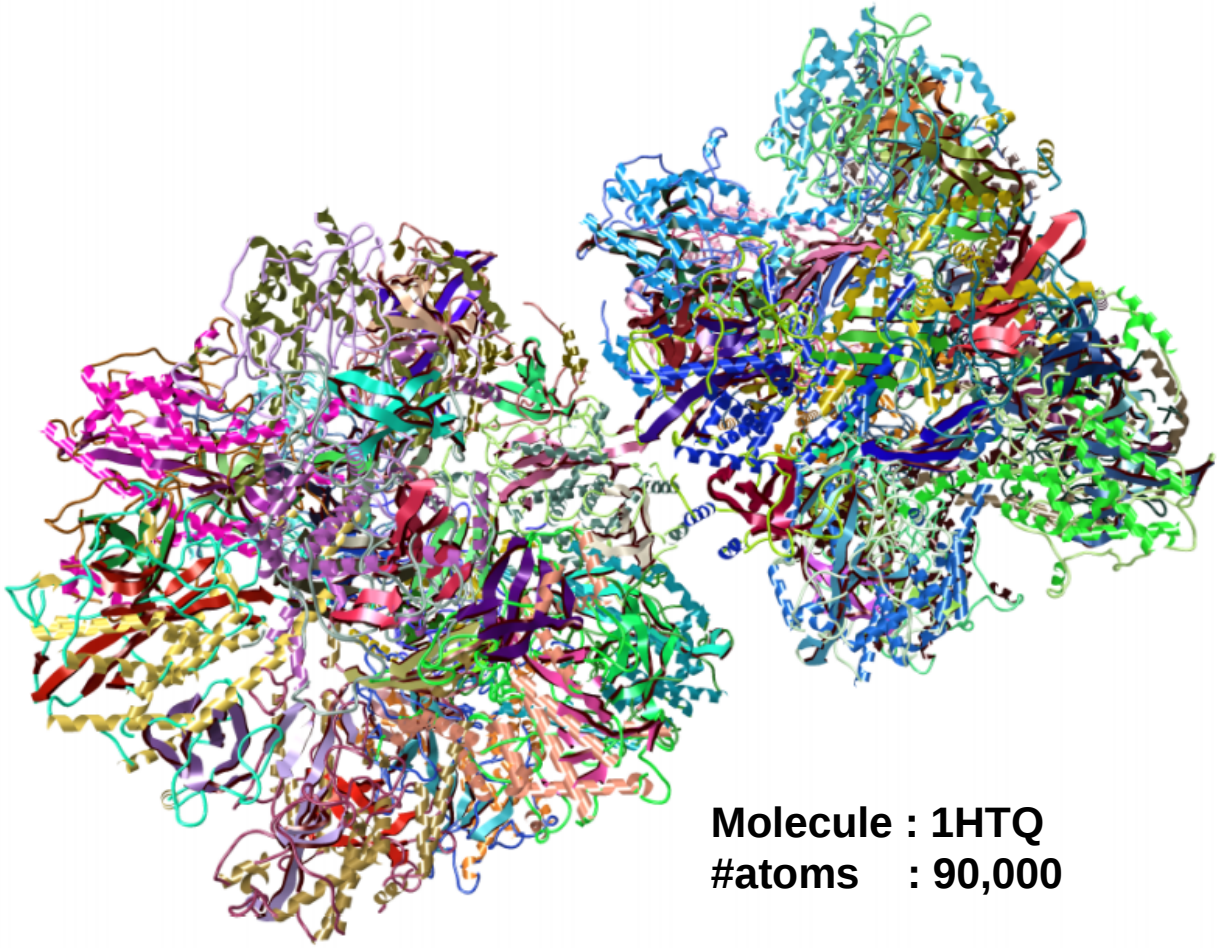
- The Cα atoms in each residue of the chain are used as control points
- Cut planes are determined by the preceding and succeeding line segments



Helical Impostors

- Modify secondary stage of cylinder Impostor
- Use radius and the pitch to discard fragments not on the helix



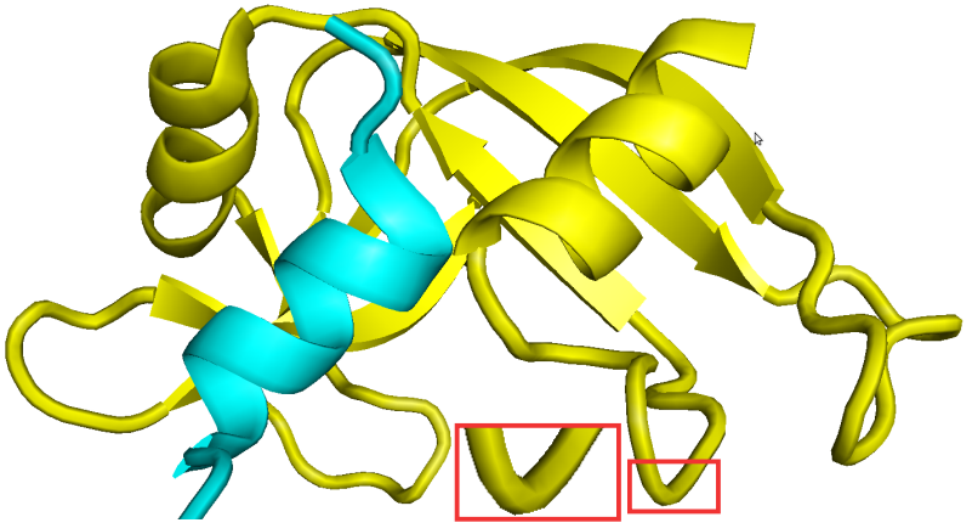


Molecule : 1HTQ
#atoms : 90,000

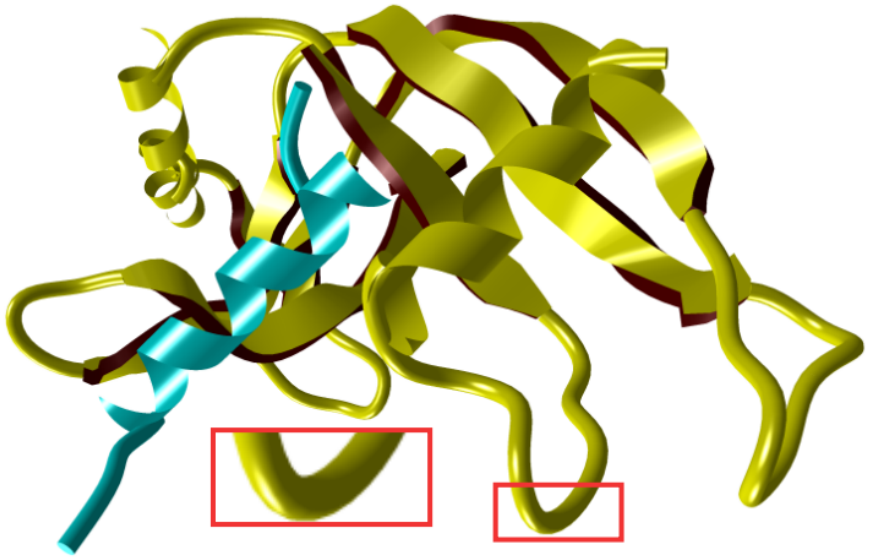
Secondary structure using Impostors

- Impostors for helices and tubes
- Accelerated rendering of spline surfaces for β-sheets
  [Krone et.al, TPCC 2008]

Results



VMD



ProteinVis

Qualitative Comparison

Avoiding Artifacts : Spline twisting

A comparison of ProteinVis against other popular protein viewers

Viewer	Space-fill	Ball-stick	Back-bone	Alpha-helices	Secondary structure
VMD 1.9.1	2.38	2	25	-	35
PyMol 1.4	45	10	-	-	21
ProteinVis	52	60	68	460	83

Molecule : 1AON
#atoms : 58,000

Quantitative Comparison-1

Better frame Rates : Shown here by comparing proteinVis against other popular protein viewers

Molecule	#atoms	ProteinVis	Hybrid [Krone et.al]
1OGZ	943	870	550
1VIS	2481	556	200
1TII	5478	274	150
1AF6	10,049	160	100
1AON	58,673	34	10
1HTQ	90,000	21	-

Hardware : Nvidia GTX 8800
Memory : 768MB

Quantitative Comparison-2

Better frame Rates : compared with hybrid implementation of [Krone et.al, TPCC 2008]

Conclusions

Contributions

- 2-step framework
- Helical Impostors
- Non-Parallel Caps
- Extension to tubes

Results

- Pixel precise rendering
- 1.5x - 2x speedup for secondary structure representation
- Up to 30x speedup for ball-stick representation
- Much better memory utilization - by a factor of 1,000

Future work

- Application to dynamic data

Acknowledgements

Department of Science and Technology
Indian Academy of Science
Dr. Patrice Koehl

Thank you

Type	#Atoms	#Triangles Triangulation	#Triangles Impostering
Alpha-Helix	58,673	8,51,208	1,674
Tubes	58,673	38,36,412	19,18,206

Table-1

Type	#Atoms	Memory Triangulation	Memory Impostering
Alpha-Helix	58,673	9,975.01 KB	13.08 KB
Tubes	58,673	44,958 KB	29,972 KB

Table-2

Triangulation Vs Impostoring :

Table-1 : Comparison based on number of triangles used.

Table-2 : Comparison based on Memory usage in GPU