Text - Image

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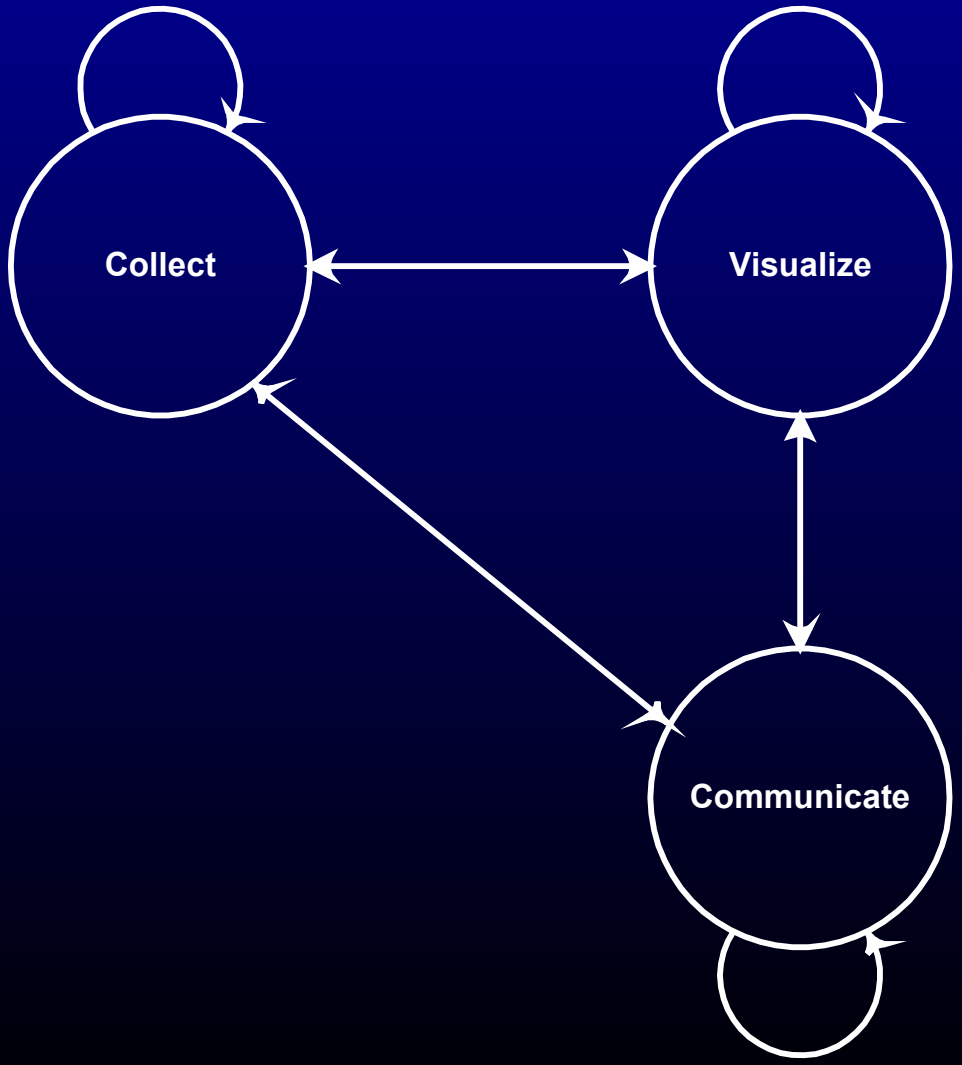
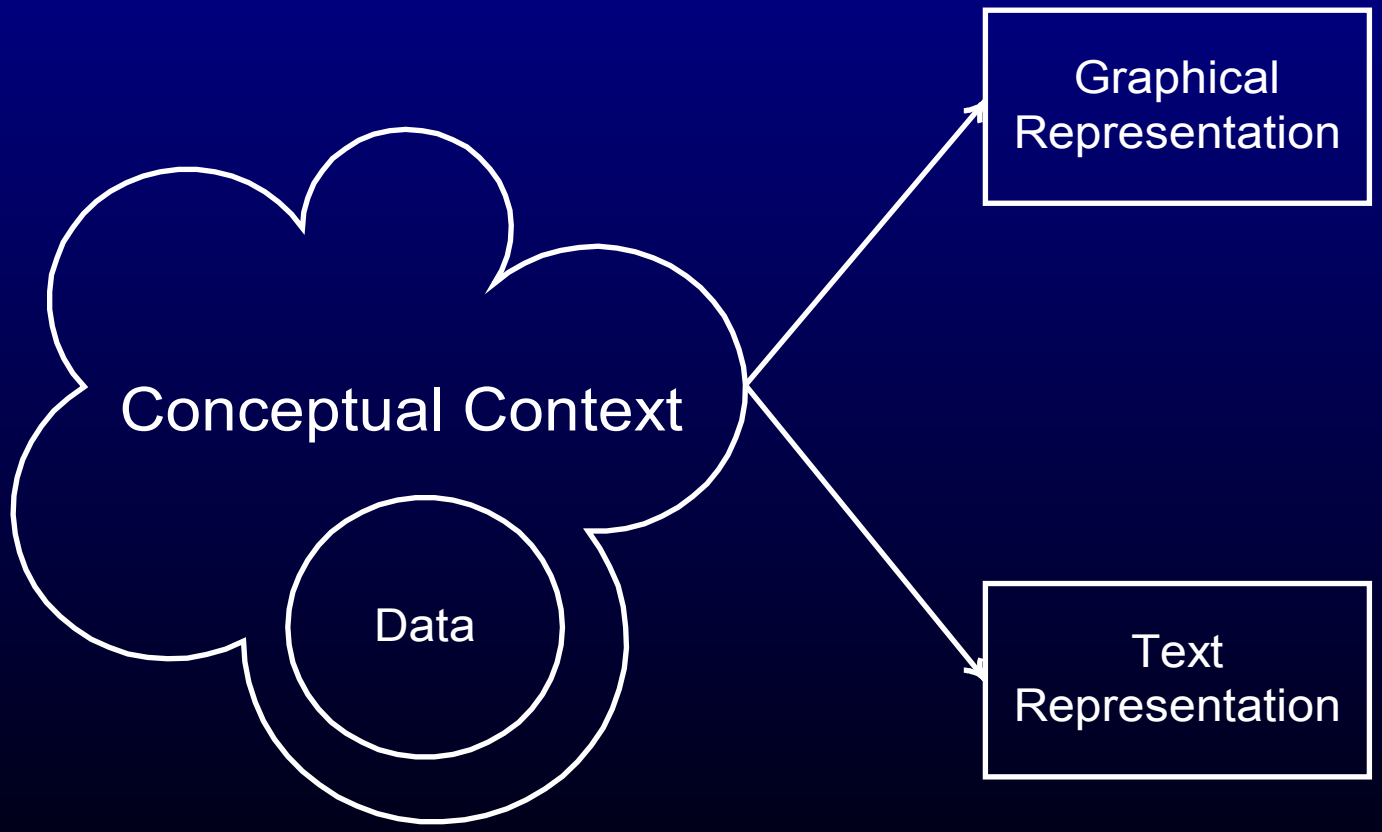
Information Communication



Information Communication



What information is communicated?

How is information communicated?

How much information is communicated?

How well is information communicated?

Vase of Flowers , 1689

Rachel Ruysch

What information is communicated?

How is information communicated?

How much information is communicated?

How well is information communicated?

CAVE, Center for High Performance Computing and Visualization (HPC/V)

University of Groningen

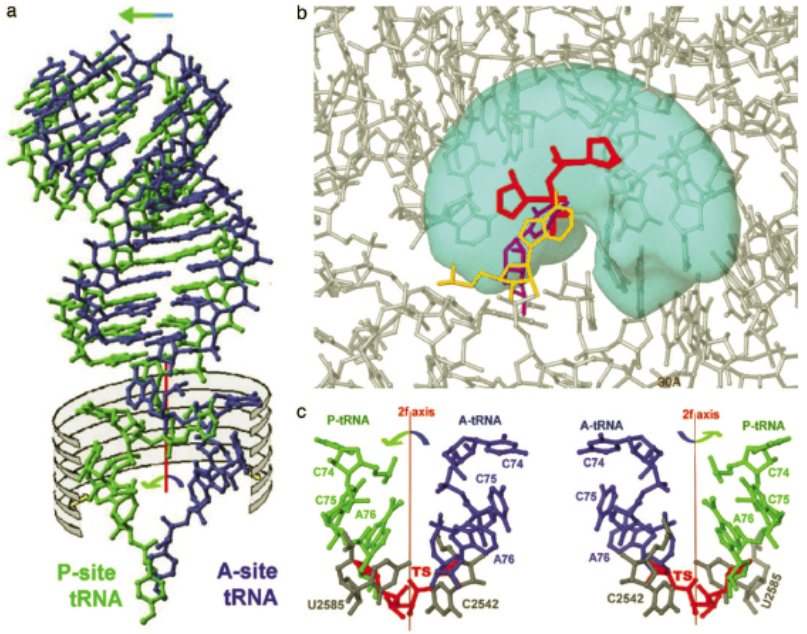


Fig. 2. The TS position within the volume occupied by the rotatory motion in the PTC of the ribosome. (*a*) A schematic presentation of the combined linear and rotational motions involved in the passage of the A-site tRNA from the A site to the P site. The 2-fold symmetry axis is shown in red. The apparent overlap of the two tRNA stems is a result of the specific view (diagonal toward the back of the paper plane), chosen to show best the concerted motions. (*b*) The approximately orthogonal view of the rotatory motion shown in *a*, looking approximately down the 2-fold symmetry axis, together with the TS, formed after 45° rotation (A site to P site) within the PTC of the ribosome. The transparent cyan "cloud" shows the entire rotatory space, as was simulated every 15° of the rotation. The ribosomal nucleotides are shown in gray. Those below the rotatory space are shown in lighter gray. The TS is shown in dark red. Nucleotides A2602 and U2585 are colored purple and yellow, respectively. Note the marked fit between the TS position and the space provided by the ribosome. (*c*) Two views perpendicular to the 2-fold rotation axis. Shown are ends of tRNAs molecules at the P site (green), the A site (blue), the 2-fold axis (red), the TS (dark red), and the nucleotides C2452 and U2585 (gray). The TS lies at its best position between the A- and P-site tRNAs. (*Left*) View from the subunit interface. (*Right*) View from the PTC rear wall.

fits with the calculated TS, as judged by the closeness of the match between the atoms of the TS sugars, and those from the tip of the A- and P-site tRNA 3′ ends that they mimic.

We have calculated the distance between the atoms of the TS and all of the nucleotides that surround it. Only nucleotides C2452 and U2585 (*Escherichia coli* numbering throughout the text) have atoms in close proximity to the TS at 45° angle of rotation. The atoms in question from C2452 do not involve bonds either "making or breaking" in the TS. However, a nitrogen atom in U2585 base protrudes into the space nearby where a C—O bond between a P-site tRNA and an amino acid is being broken in the TS. The proximity of U2585 and the TS (Fig. 2 *b* and *c*) may possibly allow it to play a role in facilitating the break of the P-site tRNA away from the elongating protein chain. The possible contribution of U2585 to elongation, rather than to peptide-bond formation and the remoteness of A2451 from the TS, are in accord with recent findings that ruled out the critical catalytic contributions of these nucleotides to single peptide-bond formation performed by *in vitro*-assembled ribosomes (12). Hence, the possible involvement of U2585 in elongation remains to be investigated further.

Discussion

Our goal was to investigate the formation of the peptide bond as it occurs within the ribosome. In particular, we studied the energy and geometry of the amino acid and the peptidyl that play a major part in peptide-bond formation while attached via ester bonds to the tRNAs at the A site and P site of the ribosome, respectively. We have chosen the 50 atoms we considered as the most important players in peptide-bond formation. Within that choice, and the quantum mechanics of density functional theory (DFT), we have computed a molecular structure and energy that

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A. Gindulyte, et al. 2006. "The transition state for formation of the peptide bond in the ribosome," *PNAS* 103, 36, pp. 13327–13332.

Information Communication Chasm (1)

- Text-rich Media (e.g. Scientific Journals)
  - *Text controls narrative*
  - *Images used as illustrations*
  - *Author of text sets communication context*
- Visualization Software
  - *Dynamic imagery*
  - *Text used as annotations*
  - *Narrative?*
  - *Open communication and collaboration*

Information Communication Chasm (2)

- How do we integrate text and visualization?
  1. *Text within visualization?*
  2. *Visualization within text?*
  3. *Other?*

Integrating Text and Visualization

Text within Image Space

- Positive Aspects
  - *Text and image occupy same logical and representational space*
  - *Text becomes a graphical object and inherits all relevant transforms*
  - *Text and image have direct access to data objects*

Integrating Text and Visualization

Text within Image Space

- Negative Aspects
  - *Text is a graphical component that competes with or complements imagery*
  - *Large blocks of text can obscure imagery*
  - *Text and graphics processed in different parts of brain*

Integrating Text and Visualization

Image within Text Space

Traditional Hypermedia

- *Static text and image dynamically linked*
- *Embedded visualization software and other media coexist*
- *Narrative text, image, and software not necessarily synchronized*