Cellular signal transduction involves a transport step. This leads to a concentration gradient of signaling molecules between plasma membrane and nucleus. Agent-based simulations produce this gradient by tracking individual proteins through a virtual cell. How can the gradient be visualized? Biologists are used to concentration plots and single proteins are difficult to spot. Where is the highest concentration? Which proteins are close to the nucleus? Do proteins accumulate?

**Motivation**

- Cellular signal transduction involves a transport step. This leads to a concentration gradient of signaling molecules between plasma membrane and nucleus.
- Agent-based simulations produce this gradient by tracking individual proteins through a virtual cell.
- How can the gradient be visualized?
- Biologists are used to concentration plots and single proteins are difficult to spot.
- Where is the highest concentration?
- Which proteins are close to the nucleus?
- Do proteins accumulate?

**Goals**

- Bridge the gap between concentration profile and discrete protein positions.
- Compute 3D concentration map from signal proteins.
- Use volume rendering for visualization.
- Investigate signal transport in the MAPK pathway (mitogen activated protein kinase).

**From Isolated Particles to a Contiguous Representation**

- A density field is reconstructed from discrete particle distributions.
- A filter kernel with support is applied to each particle.
- Accumulated densities are stored in a high-resolution uniform grid.
- Volume is built slice-by-slice on the graphics hardware (GPU).
- Volume rendering is used in a subsequent step for visualization.

**Signal Transduction in a Virtual Cell**

- Simplified mitogen activated protein kinase (MAPK).
- Receptors phosphorylate signal proteins to MAPKp.
- MAPK is transported to the nucleus.
- Phosphatases can deactivate signal proteins.
- Virtual cell is composed of microtubules, receptors, signal proteins, MAPK, phosphatases, plasma membrane, and nucleus.

**Continuous Protein Concentration**

- Areas with high concentrations are easy to spot.
- Considers spatial aspects in contrast to the traditional concentration profiles.
- Allows tracking of the signaling front.

**Signal Transport in the MAPK pathway**

- Simulation with asymmetric cell.
- Diffusion:
  - Uniform distribution.
  - Signal is attenuated toward nucleus.
- Motorized transport along microtubules:
  - Clustering along cytoskeleton.
  - Overcompensates signal deactivation.

**Results**

- On current graphics hardware (GPU) computation is possible in real-time without precomputations.
- 10-30 frames per second.
- Interactive exploration crucial for 3D data.
- Animations or time series necessary for time-dependent data.
- Data set: Simulation of MAPK (30,000 particles).

**References**