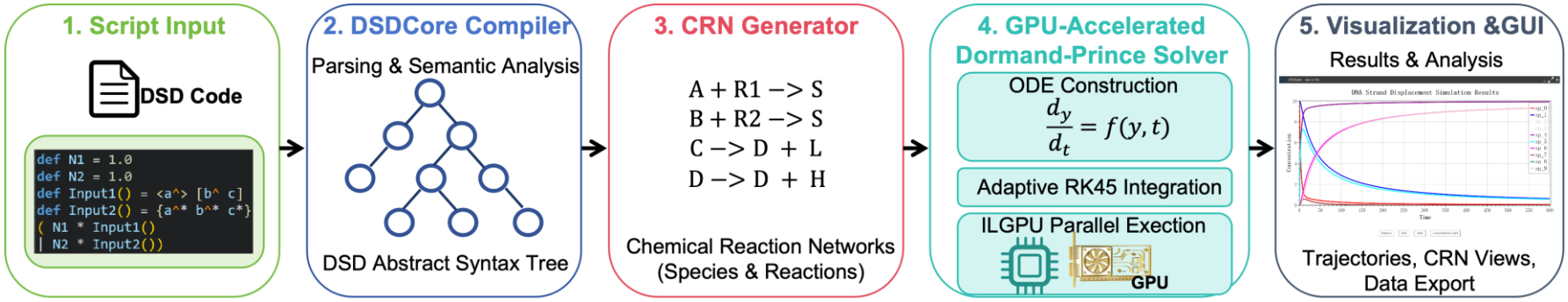
DSDStudio: A GPU-Accelerated General-Purpose DSD Simulation Software

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Problems & Ideas

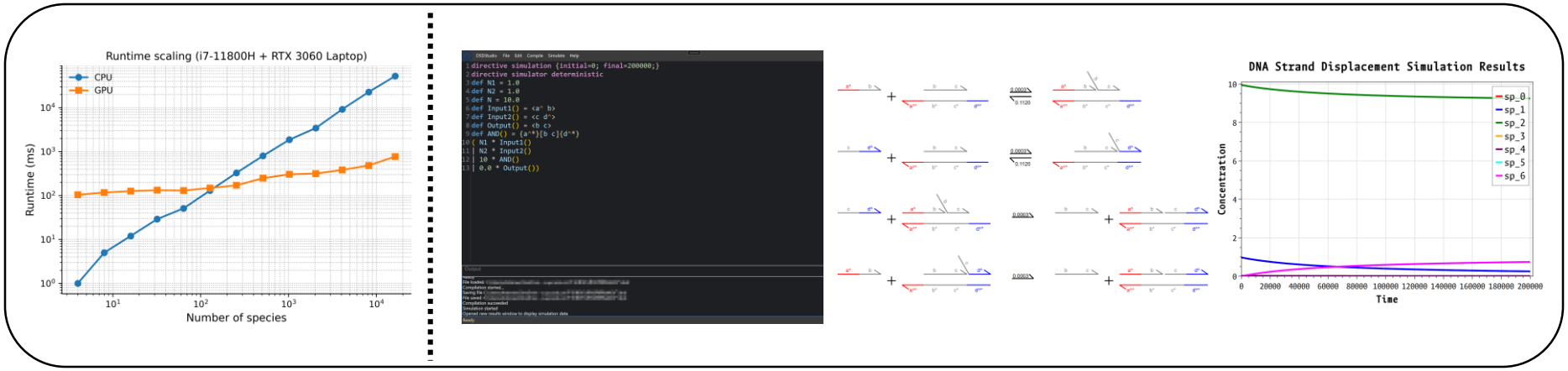
- Problems of conventional DSD simulation approaches:
  - Exponential growth in molecular species and reactions as circuit complexity increases leads to combinatorial explosion.
  - Existing CPU-based simulators evaluate reaction rates sequentially, creating severe computational bottlenecks for large-scale systems.
- Ideas: A GPU-accelerated general-purpose DSD simulation framework that takes both reaction network generation and adaptive ODE solving into account within a unified workflow.



System architecture and workflow, including DSD script parsing, chemical reaction network generation, GPU-accelerated Dormand--Prince (RK45) solving, and result visualization.

Main Contributions

- Contributions:
  - A GPU-accelerated DSD simulation framework (DSDStudio) that integrates a domain-specific compiler, CRN generation, and adaptive Dormand–Prince ODE solving into a unified workflow, achieving up to 67.7× speedup on systems with 16,384 species;
  - A parallel rate evaluation scheme using ILGPU that maps species-wise calculations to GPU threads with flattened memory arrays, together with an MVVM-based GUI providing SVG visualization, LaTeX ODE rendering, and concentration-time plotting, validated against Visual DSD on three canonical DSD circuits.



Simulation results. The maximum reported speedup of DSDStudio reaches 67.7× at 16,384 species (left). A two-input AND gate simulation includes: DSD code defines input strands and gate complex; DSDStudio automatically generates the reaction network; and the output concentration is shown (right).