Executive Summary

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This report investigates the integration of numerical Gaussian Processes (GPs) for solving linear partial differential equations, focusing on the Burger's equation and the wave equation. The study combines GP methodology with finite difference time-stepping methods to create a hybrid approach that offers both numerical solutions and uncertainty quantification.

1.1 Key Findings

1. **Uncertainty Quantification:** GPs provide probabilistic solutions, offering valuable insight into the uncertainty of predictions, especially when initial or boundary conditions are imprecisely known.
2. **Linear Transformation Property:** The study leverages the fact that linear transformations of Gaussian Processes remain Gaussian Processes, allowing for iterative predictions based on initial data.
3. **Kernel Selection:** The choice of kernel function significantly impacts solution quality. For the Burger's equation, a non-stationary arcsine kernel outperformed the standard RBF kernel.
4. **Error Propagation:** GPs naturally propagate uncertainties through time, with uncertainty accumulating at each step, dependent on the initial data's error.
5. **Computational Challenges:** While effective, GP methods face computational limitations due to $O(n^3)$ time complexity, potentially restricting their application to large-scale problems.

Methodology

This project implemented numerical GP solvers using the GPJax library, integrating them with finite difference time-stepping methods such as backward Euler and trapezoidal rule. The approach achieved accurate predictions of wave behavior within 1 second, using time steps ranging from 0.001 to 0.01.

Implications

This project serves as a proof of concept that numerical Gaussian Processes,i.e. GPs, combined with finite difference methods, can effectively solve partial differential equations. The uncertainty estimation provided by this approach is a unique feature not achieved by traditional finite difference methods alone.

Future Directions

Further research should focus on:

- Improving computational efficiency, possibly through sparse GP approximations
- Extending the approach to more complex systems such as coupled PDEs or higher-order equations
- Exploring applications in fields where uncertainty quantification is crucial

In conclusion, this project demonstrates the potential of GPs in scientific computing, opening new avenues for research in various fields of science and engineering where both numerical solutions and uncertainty quantification are important.