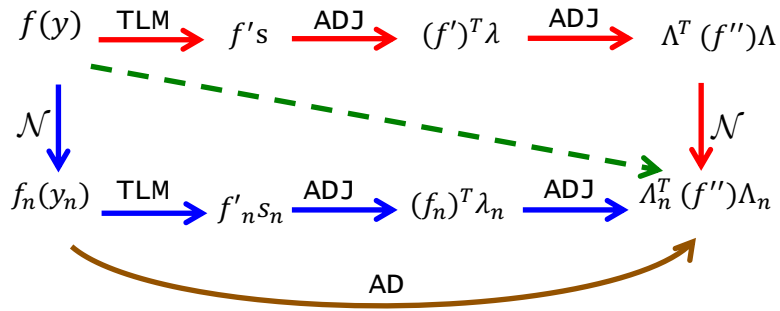


# New second-order sensitivity analysis tools are being developed for PDE-constrained optimization



Schematic illustration of **discretize-then-differentiate**, **differentiate-then-discretize** and **automatic differentiation** approaches

## Scientific Achievement

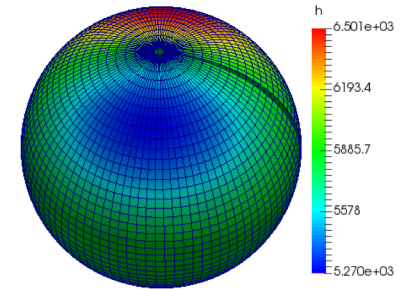
Developing new composable and scalable discrete-adjoint solvers in PETSc for time-dependent PDEs

## Significance and Impact

There is no existing ready-to-use second-order discrete-adjoint solver for large-scale time-dependent problems. The new capability enables efficient calculation of Hessian-vector products for PDE-constrained optimization

## Research Details

- The discretize-then-differentiate approach provides consistent gradients that are critical to the convergence of optimization
- Optimal adjoint checkpointing is developed to utilize the hierarchical memory on supercomputers (e.g. Theta)
- The implementation allows for multiple objective functions and integration over multiple time intervals as needed by applications in climate and power grid



Adjoint-based 4D-Var global data assimilation



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