Extending Albany to Solve PDEs on the Sphere

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Objectives

Develop a ***next-generation*** atmosphere model by leveraging Albany, a C++, parallel, implicit, unstructured-grid finite element code from Sandia National Laboratories that demonstrates ***agile components*** and enables rapid prototyping. Unique features will include embedded ***uncertainty quantification***, ***performance portability***, and a wide variety of ***discretizations***.

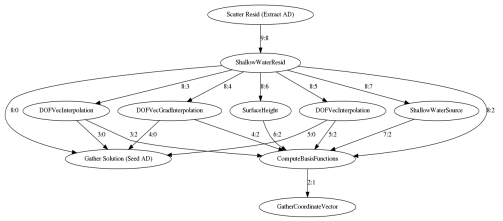
Component-Based Strategy

Component-based approach enables **rapid** development of new **production** codes embedded with **transformational** capabilities

"Components" = ☑ Libraries ☑ Software Quality Tools ☑Interfaces ☑ Demonstration Applications

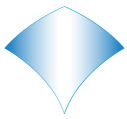
Sandia's components effort includes ~100 interoperable libraries

Graph of Finite Element Assembly Kernels



Dependency graph of finite element assembly kernels for the Shallow Water equations. By use of operator overloading-based automatic differentiation (AD), the same code base is used for implicit and explicit calculations. Most kernels shown here are general-purpose finite element calculations that were provided by Albany.

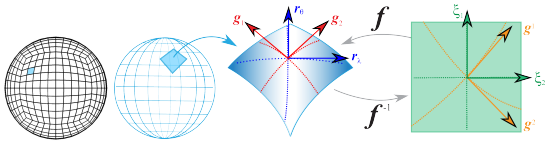
Modifications to Albany



Shell elements

Mathematically 2D elements on a 3D manifold. This will enable other applications in solid mechanics, etc.

Mapping from sphere to unit square

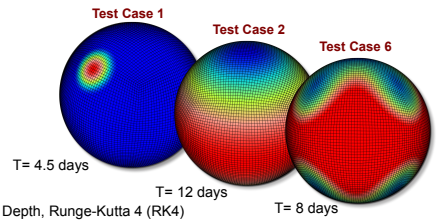


We store velocities globally using the spherical coordinate basis. In order to compute the gradient, divergence and curl, we transform to covariant, contravariant, and parametric vector bases as depicted in the figure and table.

Name	Symbols	Notes
Spherical	$\boldsymbol{r}_\lambda, \boldsymbol{r}_\theta$	Global vector basis independent of mesh, locally orthogonal, multivalued at poles
Covariant	$\boldsymbol{g}_1, \boldsymbol{g}_2$	Aligned with shell elements, non-orthogonal, components orthogonal to contravariant components, $\boldsymbol{g}_1 = \partial \boldsymbol{f}/\partial \xi_1$, $\boldsymbol{g}_2 = \partial \boldsymbol{f}/\partial \xi_2$
Contravariant	$\boldsymbol{g}^1, \boldsymbol{g}^2$	Aligned with shell elements, non-orthogonal, components orthogonal to covariant components, $\boldsymbol{g}^1 = \partial \boldsymbol{f}^{-1}/\partial \lambda$, $\boldsymbol{g}^2 = \partial \boldsymbol{f}^{-1}/\partial \theta$
Parametric	ξ_1, ξ_2	Aligned with computational element, orthogonal

Numerical Results

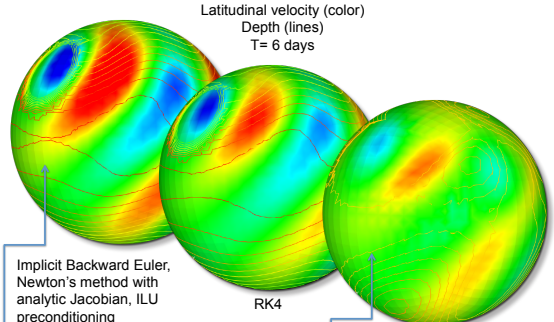
Biquadratic Finite Elements



Depth, Runge-Kutta 4 (RK4)

Test Case 5

Latitudinal velocity (color)
Depth (lines)
T= 6 days



Implicit Backward Euler, Newton's method with analytic Jacobian, ILU preconditioning

RK4

Sensitivities with respect to mountain height

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