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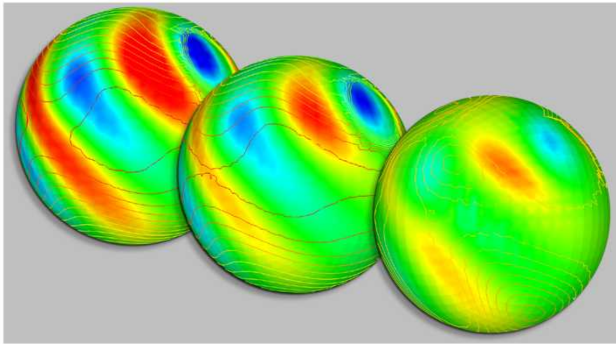

A Next-Generation Global Atmosphere Model

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ICCS 2015, Reykjavic, Iceland

Outline

Areas is a next-generation global atmosphere model funded by the Laboratory-Directed Research & Development (LDRD) program at Sandia National Laboratories. Principle next-generation capabilities include uncertainty quantification and performance portability

- Albany
- Aeras Code Suite Status
- UQ Results
  - Sensitivity
  - Concurrent Ensembles
- Performance Portability Results
- Summary

Albany

Trilinos

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Analysis Tools (*black-box*)
- Optimization
- UQ (sampling)
- Parameter Studies
- V&V, Calibration
- OUU, Reliability

Analysis Tools (*embedded*)
- Nonlinear Solver
- Time Integration
- Continuation
- Sensitivity Analysis
- Stability Analysis
- Constrained Solves
- Optimization
- UQ Solver

Linear Algebra
- Data Structures
- Iterative Solvers
- Direct Solvers
- Eigen Solver
- Preconditioners
- Matrix Partitioning

Architecture-Dependent Kernels
- Multi-Core
- Accelerators

Composite Physics
- MultiPhysics Coupling
- System Models
- System UQ

Mesh Tools
- Mesh I/O
- Inline Meshing
- Partitioning
- Load Balancing
- Adaptivity
- Remeshing
- Grid Transfers
- Quality Improvement
- DOF map

Utilities
- Input File Parser
- Parameter List
- Memory Management
- I/O Management
- Communicators

PostProcessing
- Visualization
- Verification
- Model Reduction

Mesh Database
- Mesh Database
- Geometry Database
- Solution Database

Local Fill

Discretizations
- Discretization Library
- Field Manager

Derivative Tools
- Sensitivities
- Derivatives
- Adjoints
- UQ / PCE Propagation

Physics Fill
- Element Level Fill
- Material Models
- Objective Function
- Constraints
- Error Estimates
- MMS Source Terms

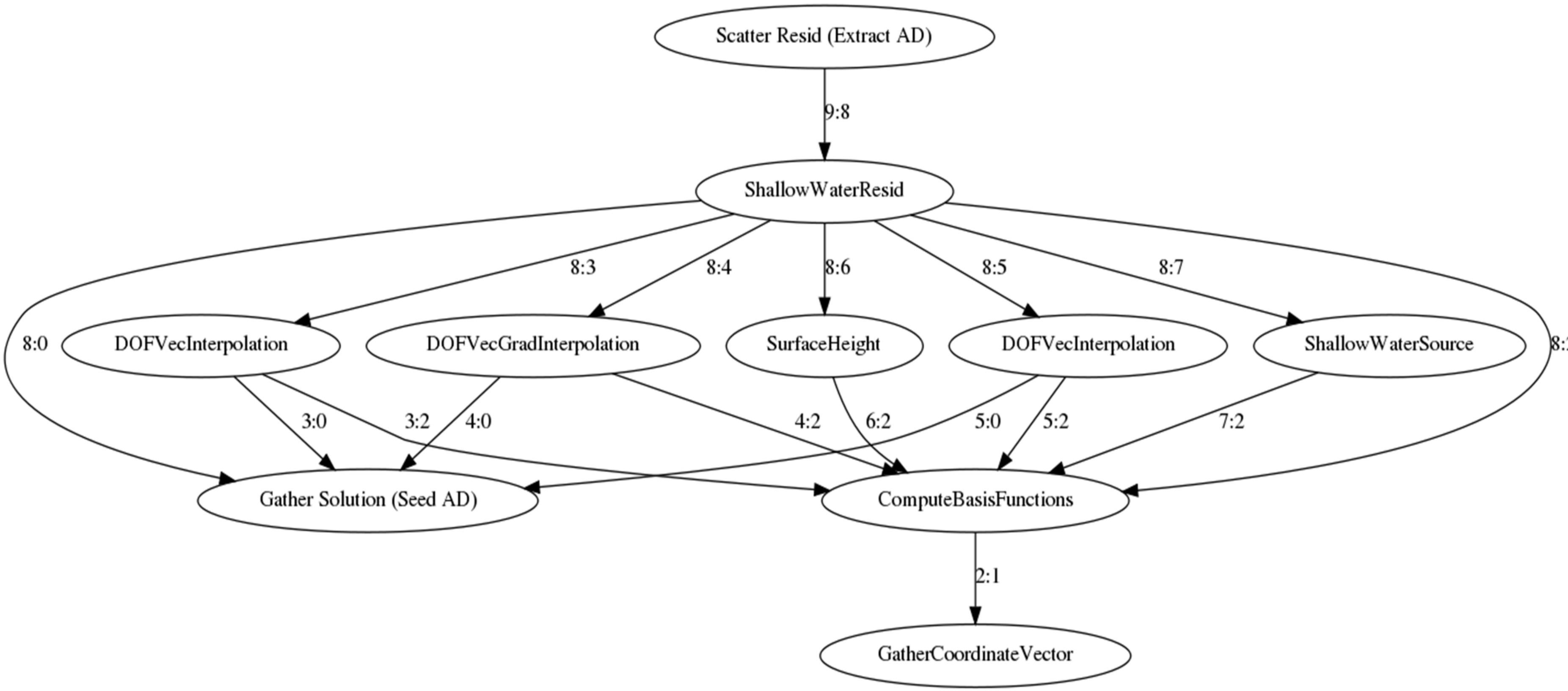
Data-Centric Algs
- Graph Algorithms
- SVDs
- Map-Reduce
- Linear Programming
- Network Models

Software Quality
- Version Control
- Regression Testing
- Build System
- Backups
- Verification Tests
- Mailing Lists
- Unit Testing
- Bug Tracking
- Performance Testing
- Code Coverage
- Porting
- Web Pages
- Release Process

Current Albany Applications

- AMP – additive manufacturing
- ATO – topology optimization
- Aeras – global atmosphere model
- FELIX – ice sheet model
- GOAL – goal-oriented adaptation
- Hydride – nuclear fuel cladding model
- LCM – laboratory for computational mechanics
- MOR – model order reduction
- QCAD – quantum device model

Albany: Dependency Graphs



Dependency Graph for Shallow Water Finite Element Assembly

Albany: Next-Generation Capabilities

- Uncertainty Quantification
  - Leverages Dakota
  - Sampling, sensitivity analysis, parameter studies, calibration
  - Embedded techniques (automatic differentiation)
  - *Concurrent Ensembles*
- Performance Portability
  - Leverages C++ Kokkos package from Trilinos
  - Memory layout abstraction (AofS vs SofA, locality)
  - Templated meta-programming: parallel_for, parallel_reduce (templates describe an *execution space*)
  - A *programming model* as much as a software library
  - Provides automatic access to OpenMP, CUDA, Pthreads, etc.

Uncertainty Quantification for Climate

- UQ is meaningless for chaotic output variables
- Prognostic variables in climate (velocities, temperature, tracers, etc.) are chaotic
  - We run climate models to obtain *diagnostic* outputs, which are not chaotic
- ➔ We should only perform UQ calculations in climate on *diagnostic* variables
- This rules out “traditional” embedded UQ techniques, as they act upon prognostic variables
  - Embedded techniques might still be useful for short-term weather forecasting
- This essentially leaves us with “black box” sampling techniques

Concurrent Ensembles

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- Scalar is already a ubiquitous template to support automatic differentiation
- Scalar and vector quantities based on template Scalar can be "upgraded" to arrays
- This allows us to compute several models concurrently – use sampling to provide more work per computing element
- Particularly attractive for explicit time-stepping algorithms – implicit methods can have "irregular" convergence
- New capability being added to Albany with Aeras as first demonstration

Code Suite Status

- Shallow Water
  - Spectral elements
  - Sensitivities verified
  - Concurrent ensembles implemented
  - Kokkos performance portability implemented
  - Implementing hyperviscosity

$$\frac{\partial \mathbf{u}}{\partial t} = -\omega \hat{\mathbf{k}} \times \mathbf{u} - \nabla\left(\frac{1}{2}u^2 + gH\right)$$

- X-Z Hydrostatic
  - Low-order elements in x
  - Gather/scatter bug…
  - Kokkos performance portability implemented

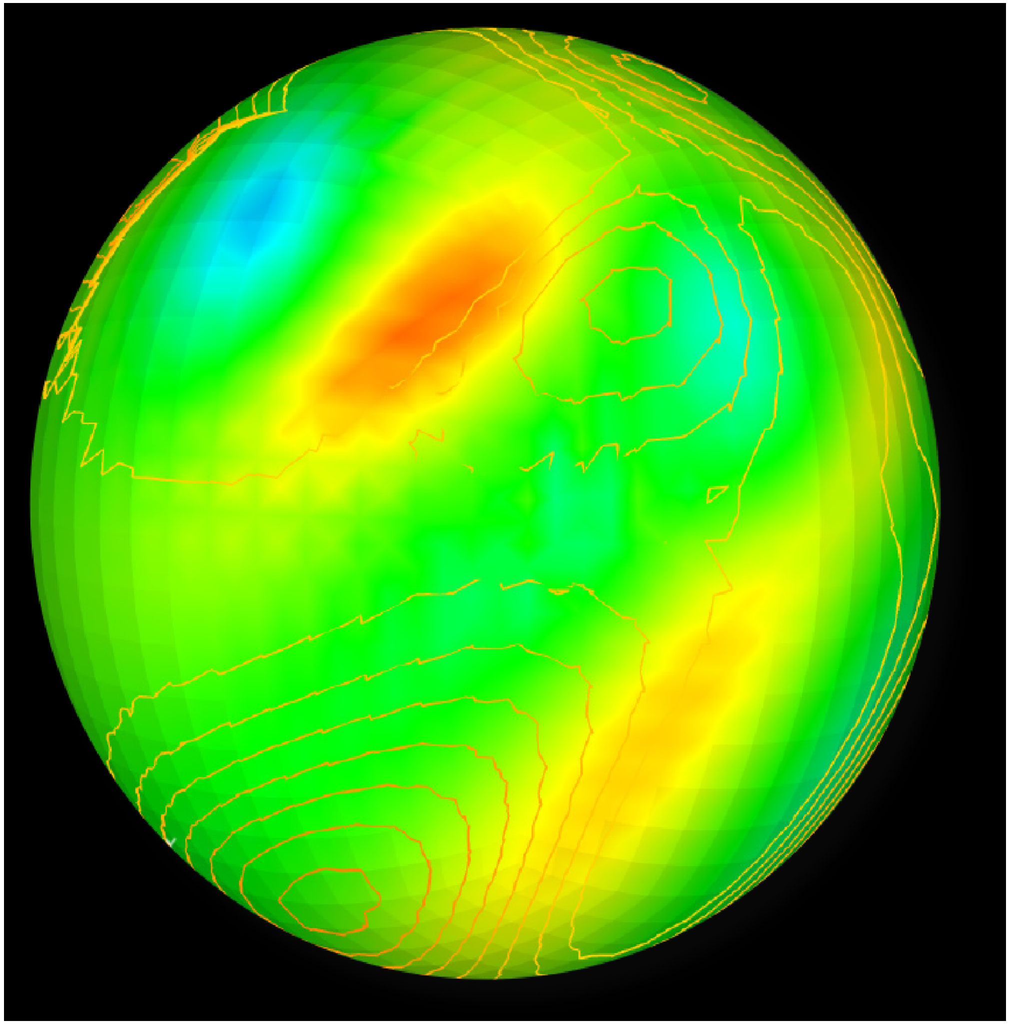
$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x}\left(\frac{1}{2}u^2 + \phi\right) + \dot{\eta}\frac{\partial u}{\partial \eta} + \frac{RT_v}{p}\frac{\partial p}{\partial x} = 0$$

- 3D Hydrostatic
  - Spectral elements
  - Gather/scatter bug…
  - Kokkos performance portability implemented

$$\frac{\partial \mathbf{u}}{\partial t} + (\zeta + f)\hat{\mathbf{k}} \times \mathbf{u} + \nabla\left(\frac{1}{2}u^2 + \phi\right) + \dot{\eta}\frac{\partial \mathbf{u}}{\partial \eta} + \frac{RT_v}{p}\nabla p = 0$$

- Cloud Model
  - Initial implementation (5 phase), awaiting hydrostatic models…
- 3D Non-hydrostatic
  - Strategy: perturbation of hydrostatic equations

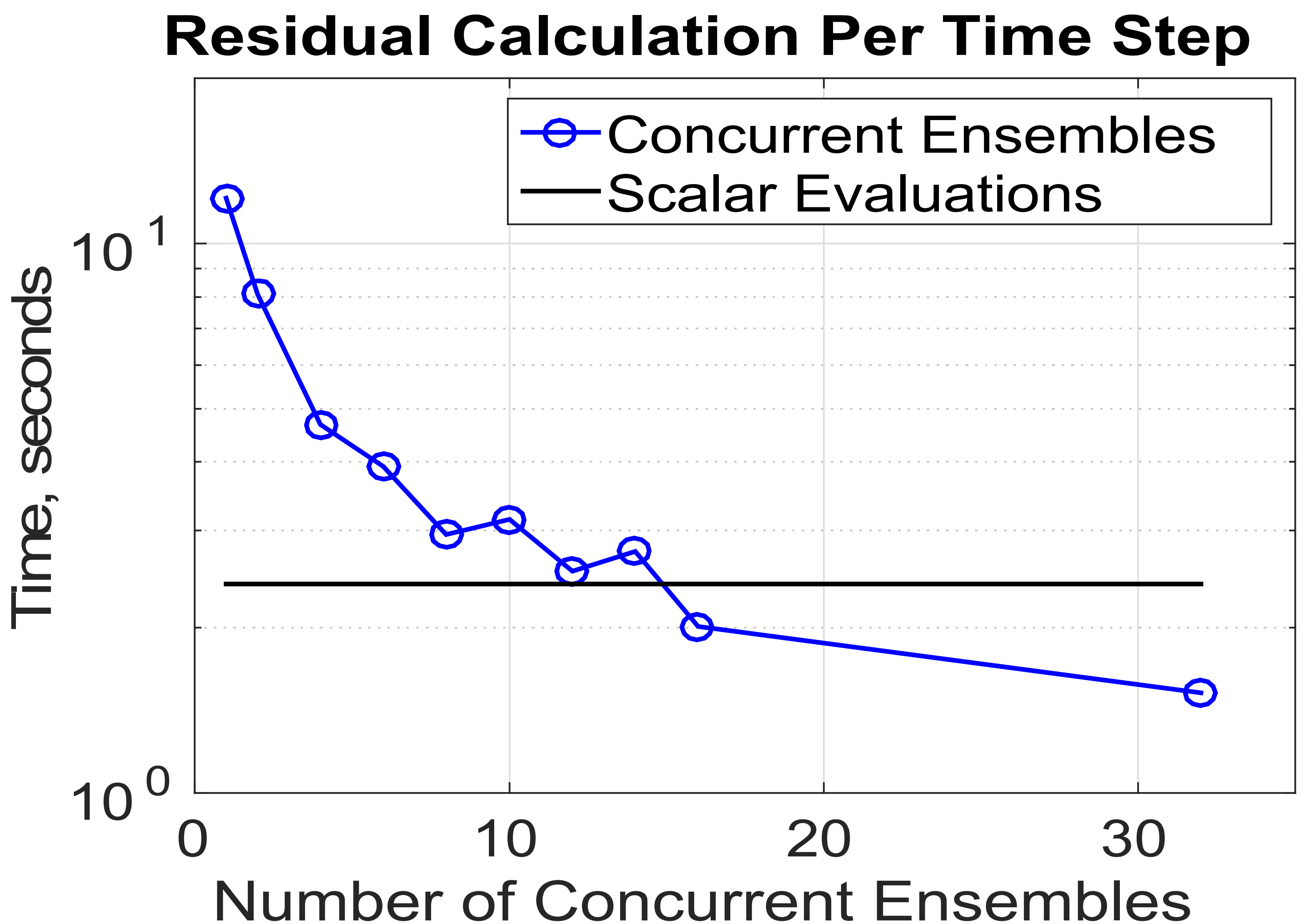
Sensitivity Calculations



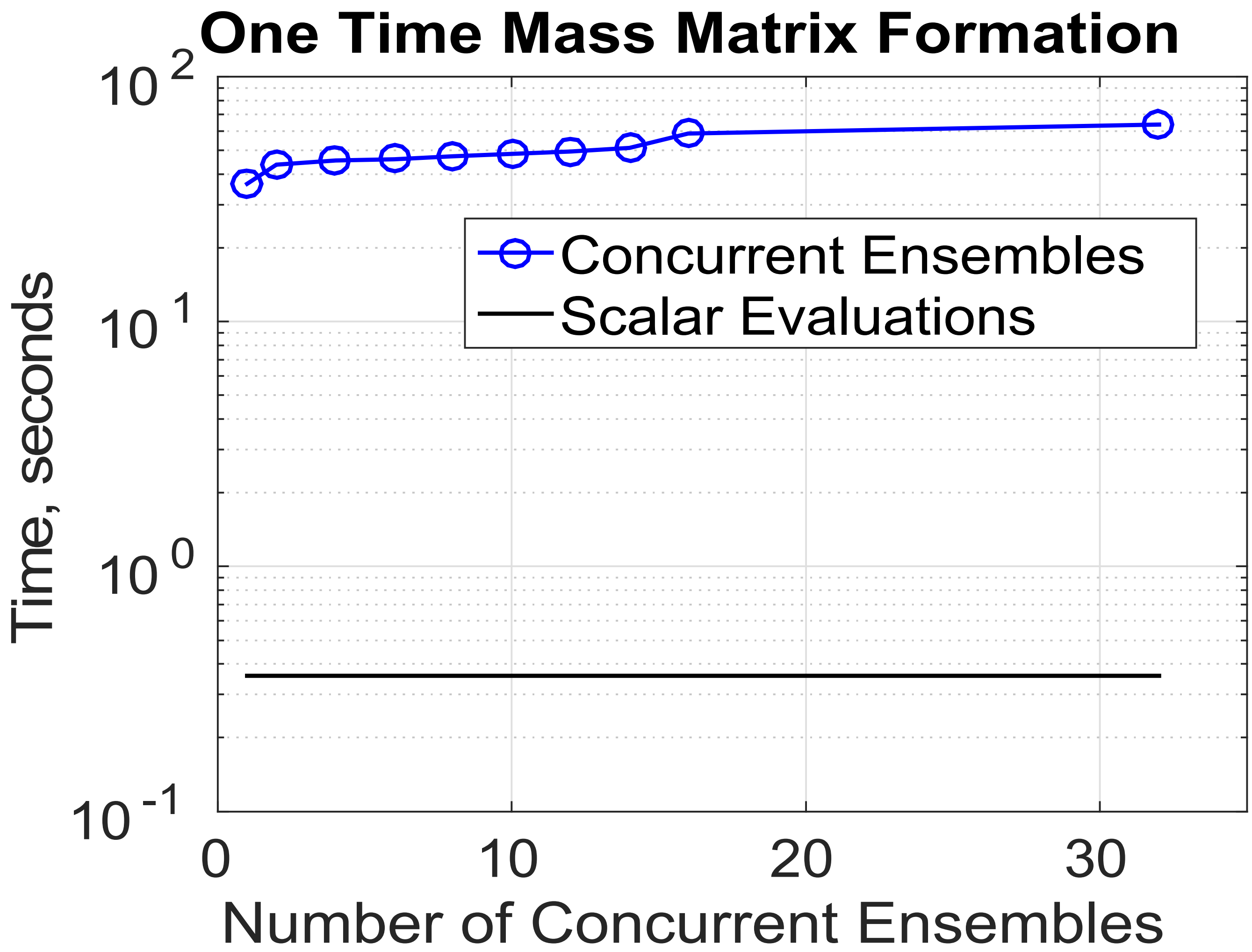
- Shallow water test case 5
- T = 6 days
- Latitudinal velocity
- Sensitivity with respect to mountain height

- Built-in Albany capability utilizing automatic differentiation
- Static capability had to be upgraded to time-dependent

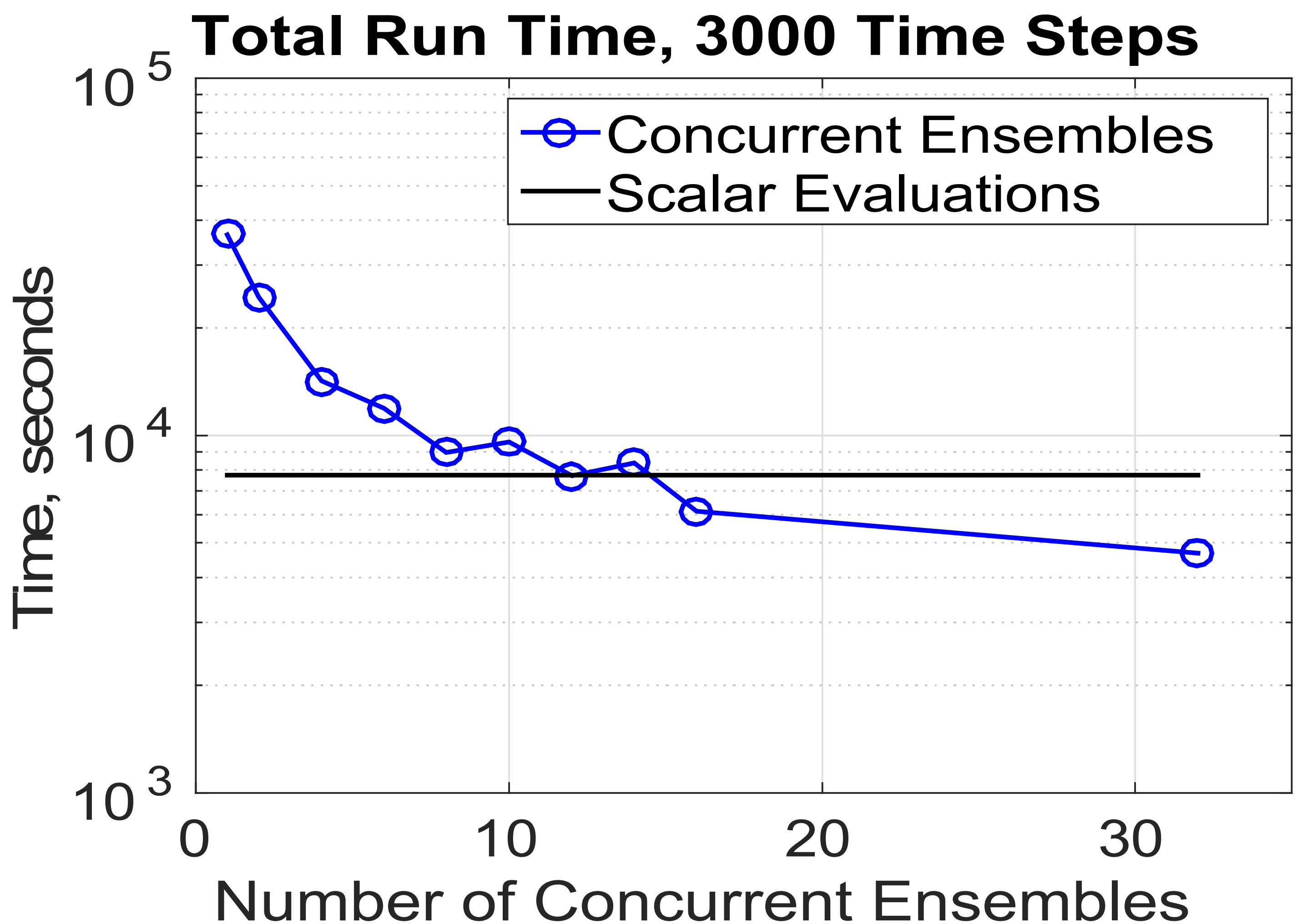
Concurrent Ensembles: Residual



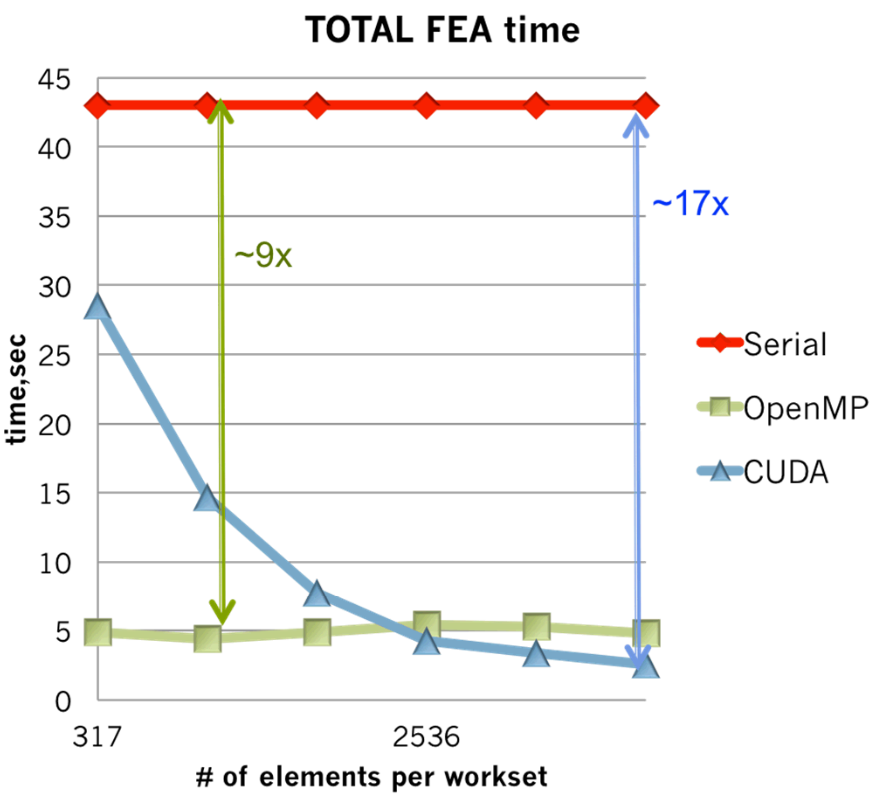
Concurrent Ensembles: Mass Matrix



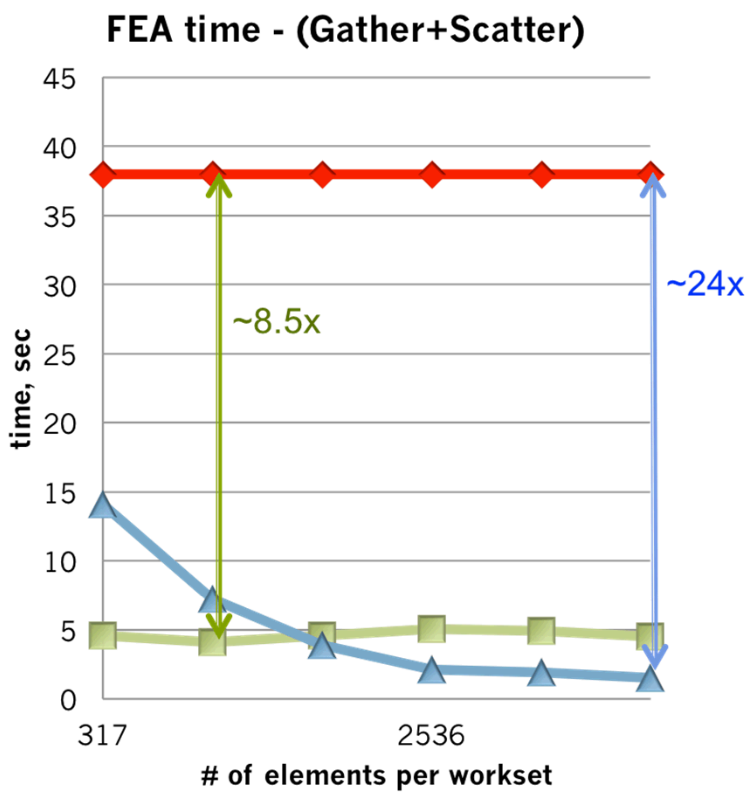
Concurrent Ensembles: Total Time



Performance Portability



a)



b)

Summary

- The Aeras project is attempting to demonstrate a next-generation global atmosphere model using cutting-edge software packages and techniques
- Next-generation features include uncertainty quantification and performance portability
- We are at roughly the half-way point of the project, with many upcoming milestones
- Concurrent ensembles have demonstrated a ~2x increase in computational efficiency for large enough sample size
- Performance portability techniques have resulted in a *single code base* for serial, threads, GPUs, etc., and have resulted in hardware-appropriate speedups