Coupling Approaches for Next Generation Architectures (CANGA)

CANGA Team Members:

P Jones, P Bochev, R Jacob, S Painter, P Ullrich, X Jiao, Z Liu,

E Constantinescu, E Coon, I Demeshko, J Guerra, H Guo, M Hernandez, S Kang, P Kuberry, V Mahadevan, B O'Neill, T Peterka, K Peterson, H Pillai, M Raj, A Reisner, D Ringo, C Sockwell, N Trask, H Wang, H Zhang

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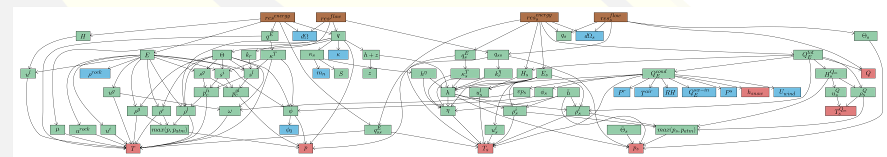
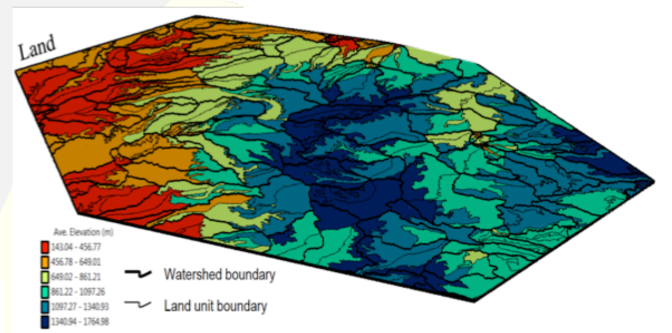
SciDAC Scientific Discovery through Advanced Computing

CANGA Project

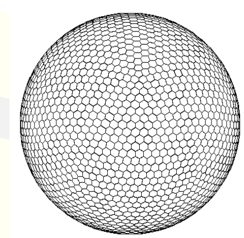
- PIGLET: Prototype Integration of Global models using Legion Execution of Tasks
  - Prototype coupler
  - Task-based components (ocean, ice, land)
  - In situ analysis

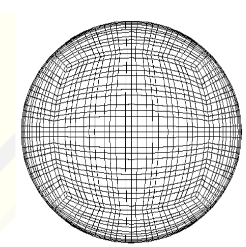


- ROO: Remapping Online-Offline
  - Irregular meshes
  - Property preserving remap
  - Adaptive on-line
  - Meshless remaps (esp. velocity)



- TIGGER: Time InteGration for Greater E3SM Robustness
  - New time integration approaches
  - Prototype/simple coupled models for testing integration



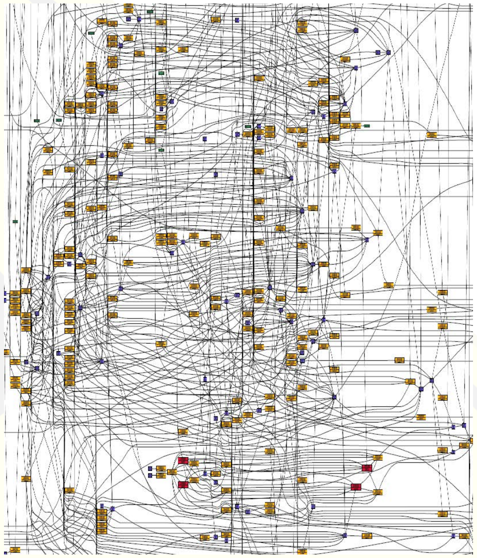


Performance Comes Through Parallelism

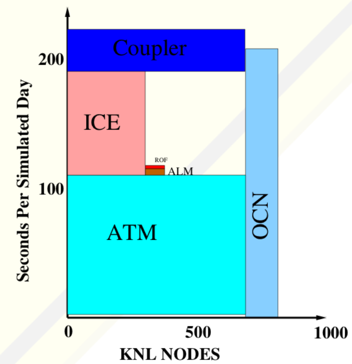
- Number of computational elements increasing
  - Multi-core CPUs
  - GPUs with substantial internal parallelism
- More hybrid elements
  - CPUs, GPUs, FPGAs, Tensor cores, burst buffers
  - configurable, custom (post-K)
- 10k-100k threads/node, variable workloads
- Programming Approaches
  - Directives (OpenMP/OpenACC)
  - Kokkos
    - Portable abstractions through template metaprogramming
    - Emphasis on data layout, indexing, some support tasking
  - 3x-10x GPU speedups (per node), addresses some portability, data access
  - Still can’t get enough work for device, esp. strong scaling regime

Asynchronous Many-Task

- Federation of tasks
  - Tasks w/ clear interfaces and intent, no side effects
  - Light-weight runtime creates DAG and schedules work
  - **Legion**, Uintah, HPX, PARSEC, others
- Computing advantages
  - Exposes more parallelism
  - Can automatically load balance
  - Fault tolerance
  - Map tasks to appropriate hardware (I/O, GPU, CPU, etc.)
- Science advantages
  - Managing complexity: to add functionality, add task to task queue
  - Treat models as collection of processes, couple at process level
  - Move away from large monolithic stove-piped components
  - Scale-aware: launch and couple tasks at appropriate time, space scales, enable more flexible time integration (requiring algorithmic change)
  - Include more of overall workflow (e.g. in situ analysis)

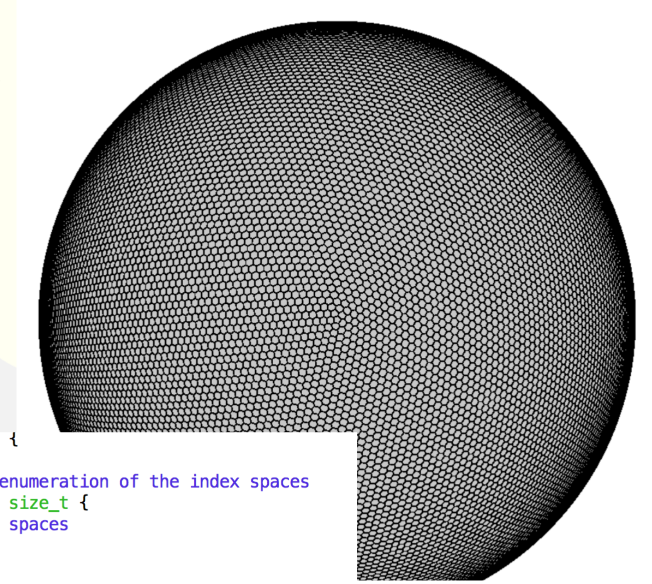


Example DAG from S3D combustion



Legion/FleCSI

- FleCSI: C++ application framework
  - Control, execution, data models
  - Runtime abstractions for AMT
    - MPI, Legion, HPX, Charm++
- Specialization layer (I. Demeshko)
  - Mesh, partitioning
  - Connectivity, owned/shared/halo
  - Performance
- Interaction with run time
  - Register fields
  - Register tasks, with fields, intent (r,w,rw)
- Launch tasks on distributed index space



```
struct index_spaces_t {

  //! The individual enumeration of the index spaces
  enum index_spaces : size_t {
    // the main index spaces
    vertices,
    edges,
    cells,
    // index spaces for connectivity
    vertices_to_edges,
    vertices_to_cells,
    edges_to_vertices,
    edges_to_cells,
    cells_to_vertices,
    cells_to_edges,
    edges_to_edges,
    cells_to_cells,
    //
    // total number of index spaces
    size = cells + 1
  };

  //! Maps an entity dimension to an index space id
  static constexpr size_t entity_map[1][3] = {
    vertices,
    edges,
    cells,
  };
```

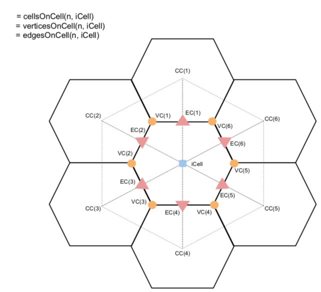
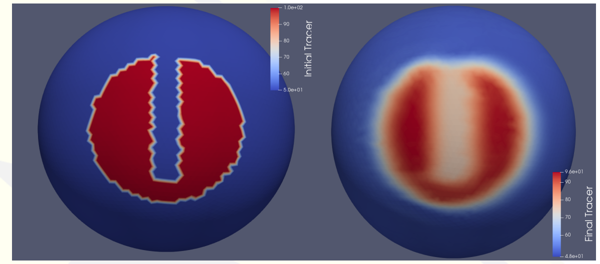
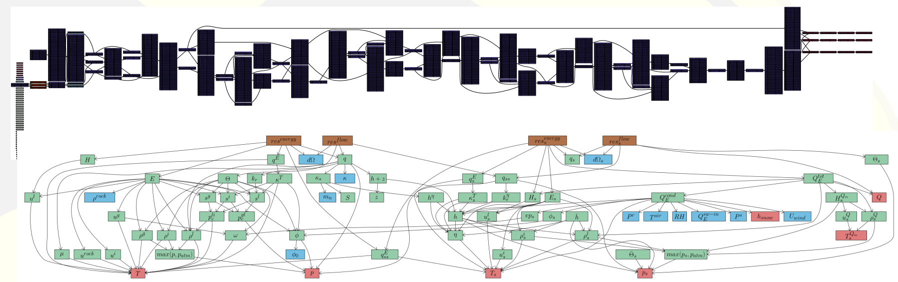


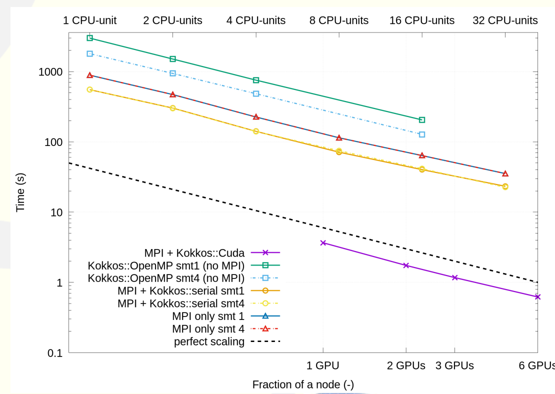
Figure 5.4: Ordering of elements relative to cells.

AMT Progress

- Coupler driver
  - Prototype working with all interfaces
  - Flesh out functions, waiting on multi-mesh
  - Future: break apart components
- Ocean mode
  - Shallow water
  - Baroclinic test case
  - Next: compare w/ MPAS
- Land
  - Extracted several kernels from ELM
  - Mini-app: drivers for Legion, Kokkos, etc.
  - Comparing performance
- In-situ analysis: Lagrangian particles

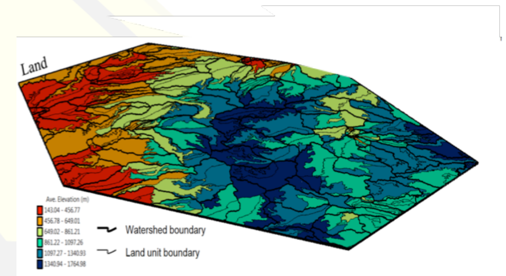




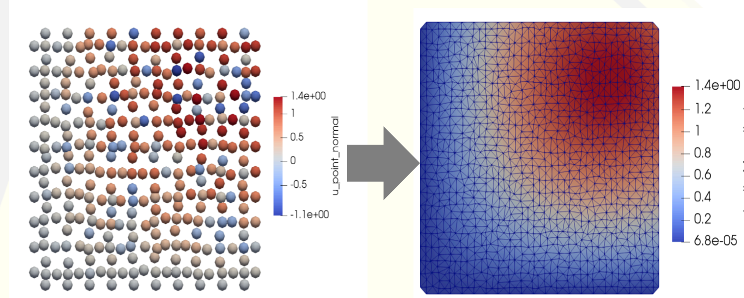


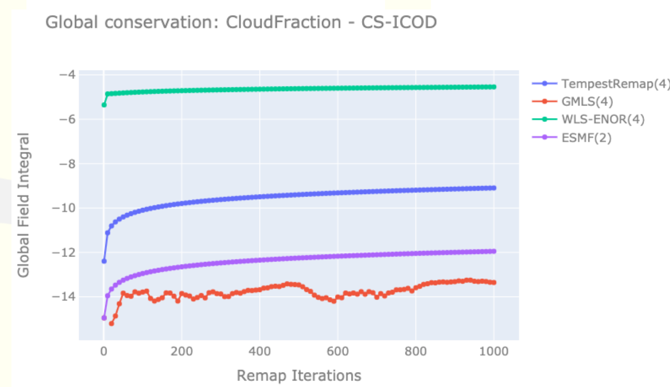
New Remapping Algorithms

- New features related to Tempest remap
  - Irregular meshes (eg watersheds)
  - MOAB integration
  - Property preservation (Conserv., bounds preserv)
  - Next: vector
- Meshless Remap
  - Remap from native field locations
  - Property preservation (as above, next: vector)
- Adaptive online remap
  - Adapt order of remap based on field properties
  - Discontinuities in fields/domains
- Test and intercomparison framework
  - Analytic form of observed fields (trunc Spher. Harm.)
  - Large range of metrics (accuracy, convergence, conservation, extrema, others)



Data Transfer from Face Elements (RT) to a nodal finite element basis





Time Integration

- New time integration schemes and analysis
  - Goal of consistent, accurate schemes with no iteration of components
  - Bulk-IFR, ImEx, Heterogeneous
  - SNL, ANL/OSU groups
- Simpler prototype coupled systems
  - Advection, diffusion equations
  - Coupling using bulk formulae at interface
- Analysis of existing E3SM coupling

Atmosphere/ocean tracer

$$\dot{T}_a + \frac{\partial}{\partial x}(u_a T_a) = \frac{\partial}{\partial z} K_a \frac{\partial T_a}{\partial z}$$

$$K_a \frac{\partial T_a}{\partial z} = K_o \frac{\partial T_o}{\partial z} = \alpha (T_a - T_o) \qquad \Gamma$$

$$\dot{T}_o + \frac{\partial}{\partial x}(u_o T_o) = \frac{\partial}{\partial z} K_o \frac{\partial T_o}{\partial z}$$

Non-Iterative Methods for Ocean-Atmosphere Coupling

Bulk Interface Flux Recovery (Bulk-IFR) Coupling Method:

- Approximates interface flux of **monolithic system**
- **Schur complement** method
- Approximates flux at **current time-step** t_{n+1}
- Subsystems solved **independently** with flux as BC

Pros:

- Flux conservation
- Stability
- Consistent time discretization
- Decoupled components
- Heterogeneous time discretization

Cons:

- Schur complement is expensive (future research)

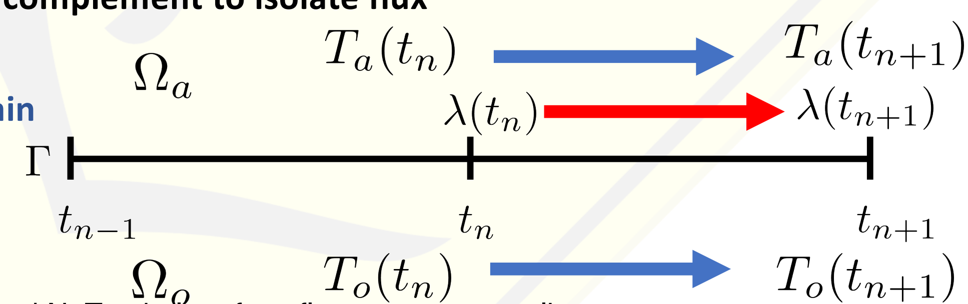
- **Step 1: Define flux as auxiliary variable**

$$\lambda = K_a \frac{\partial T_a}{\partial z} = -K_o \frac{\partial T_o}{\partial z} = \alpha (T_a - T_o)$$

- **Step 2: Define Discrete monolithic system at time t_{n+1}**

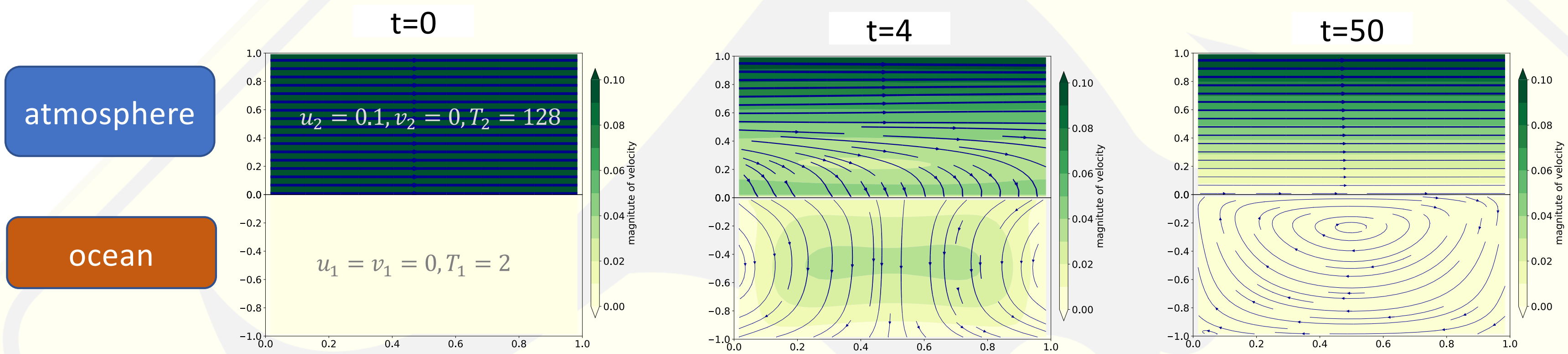
$$\begin{bmatrix} M_a & 0 & \Delta t G^T_{a,\gamma} \\ 0 & M_o & -\Delta t G^T_{o,\gamma} \\ \alpha G_{a,\gamma} & -\alpha G_{o,\gamma} & -M_\gamma \end{bmatrix} \begin{bmatrix} T_a^{n+1} \\ T_o^{n+1} \\ \lambda \end{bmatrix} = \begin{bmatrix} \Delta t f_a(T_a^n) \\ \Delta t f_o(T_o^n) \\ 0 \end{bmatrix}$$

- **Step 3: Schur complement to isolate interface DoFs**
- **Step 4: Additional Schur complement to isolate flux**
- **Step 5: Solve for flux**
- **Step 6: Update subdomain solutions independently with flux boundary conditions**



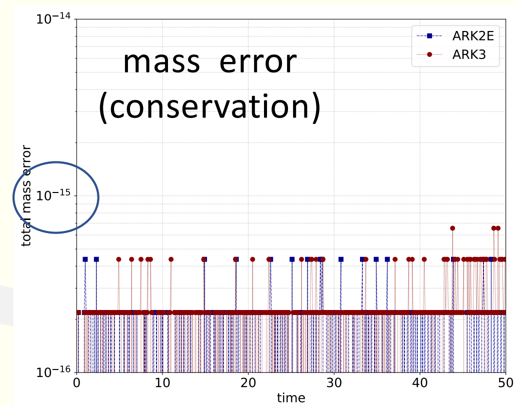
K. C. Sockwell, K. Peterson, P. Kuberry, P. Bochev, and N. Trask. Interface flux recovery coupling method for the ocean–atmosphere system. Results in Applied Mathematics, 8:100110, 2020.

ANL: Implicit-Explicit (IMEX) Coupling



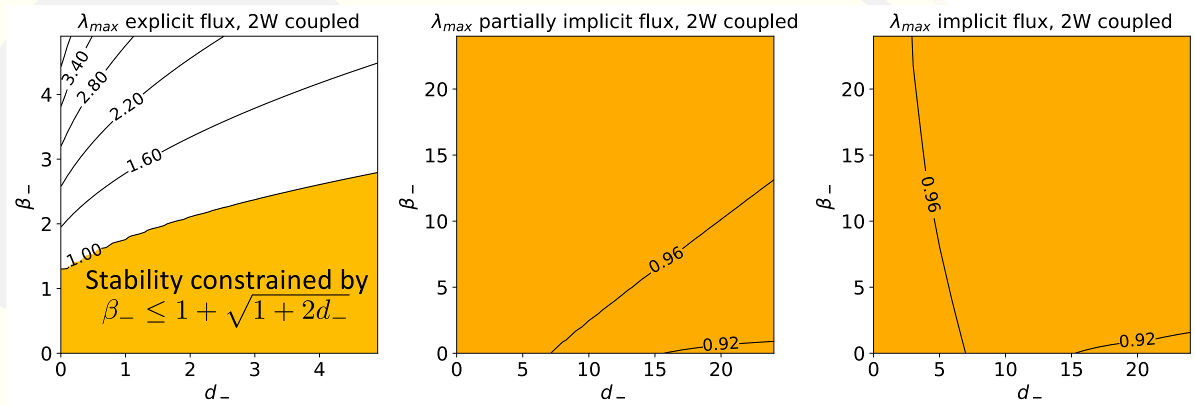
Two coupled compressible Navier-Stokes systems

- Integrate nonstiff system (ocean) explicitly and integrate stiff system (atmosphere) implicitly.
- Exchange the horizontal momentum and the heat flux across interface data under rigid-lid assumption (zero normal velocity) at every stage.
- Total mass is conserved
- High-order IMEX methods
- First-order finite volume method (interface consistency), developing high-order



TIGGER: Coupling Stability Analysis

- SNL: Nikki Plakowski, Paul Kuberry
  - Eigenvalue analysis of IFR
  - Noisy, inconclusive
- ANL: H. Zhang, Z. Liu, E. Constantinescu, R. Jacob
  - Normal mode analysis
  - Established stability theory for one-way and two-way coupled systems with bulk interface conditions. (paper published)
  - CFL-like stability condition

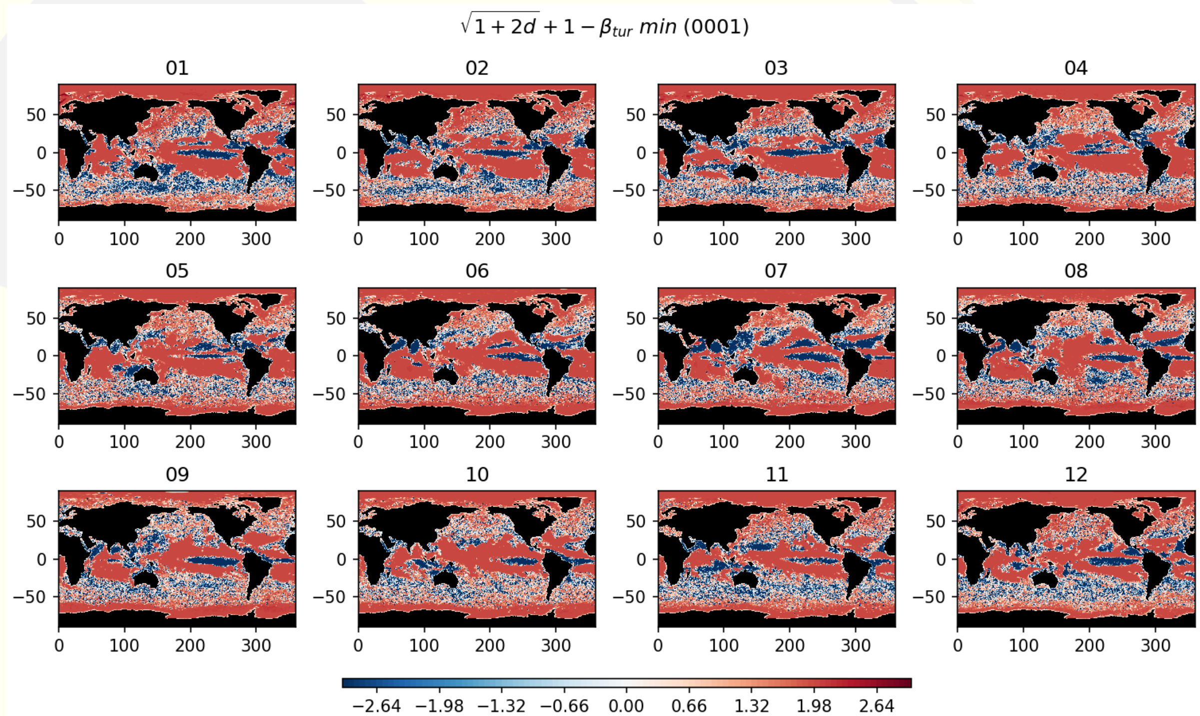


- **Hong Zhang**, **Zhengyu Liu, Emil Constantinescu, Robert Jacob,** Stability Analysis of Interface Conditions for Ocean-Atmosphere Coupling, 2019, submitted
- **Hong Zhang,** Stable time integration for coupled ocean-atmosphere models. SIAM Conference on Computational Science and Engineering, LANS Seminar, Argonne National Laboratory, November, 2019

Stability Analysis of Atmosphere-Ocean Coupling in E3SM

Analyzing and identifying regions of potential unstable coupling using the theoretical CFL-like condition

- Plot showing the minimum of the parameter. Negative value (blue) suggests potential instability during the 1-yr simulation.
- Instability appears in regions with small diffusivity and large coupling coefficient
- Significant seasonal variability: caused by that of both coupling coefficient and diffusivity



Monthly minimum of $\sqrt{1+2d}+1-\beta$ for the ocean calculated from 1-yr simulation of E3SM

Summary

- Task-parallel work progressing
  - Should understand viability soon
  - Task parallelism at some form provides some additional parallelism, flexibility
  - Mixed programming models likely
  - Continue to break up large components
- Developing new methods for coupling
  - Improved consistency, accuracy, robustness
  - Work to improve efficiency
- Developing improved understanding of coupled system
  - Stability of coupling
  - Consistency of algorithms across coupled system
  - Classifying approaches