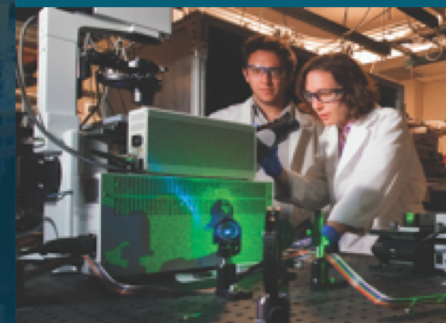
Guest Lecture Stanford ME469: Nalu Overview



PRESENTED BY

Stefan P. Domino

Computational Thermal and Fluid Mechanics

Sandia National Laboratories SAND2018-4619 PE

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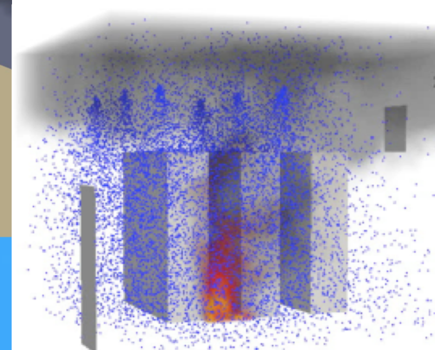
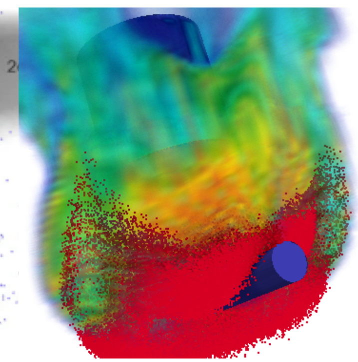
Nalu Overview: Outline

- Nalu Technology Origination: ASC
- Beyond the 32-bit Limit
- Supported Physics
- Supported Numerics
- Low- and High-order
- Moving Mesh (Sliding and Overset)
- Multiphysics:
  - Fluid Structure Interaction
  - Conjugate Heat Transfer (CHT)
  - Participating Media Radiation
- Examples
- Conclusion

Core Technology Provided to Nalu Origination: Advanced Simulation and Computing Sierra/Fuego

- Use-case characterized by a highly sooting, turbulent, reacting flow with Participating Media Radiation (PMR), Conjugate Heat Transfer (CHT), and propellant multi-physics coupling

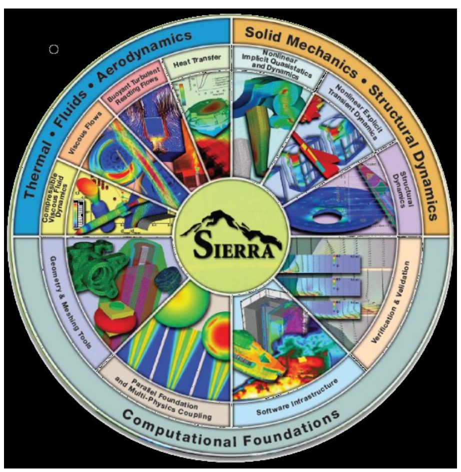


- Complex geometry has driven a generalized, hybrid unstructured discretization approach supporting Hex8, Tet4, Wedge6, and Pyramid5 elements in addition to arbitrary promotion of Hex8 to Hex27, Hex64, etc.

Goal: Beyond 32-bit Computing

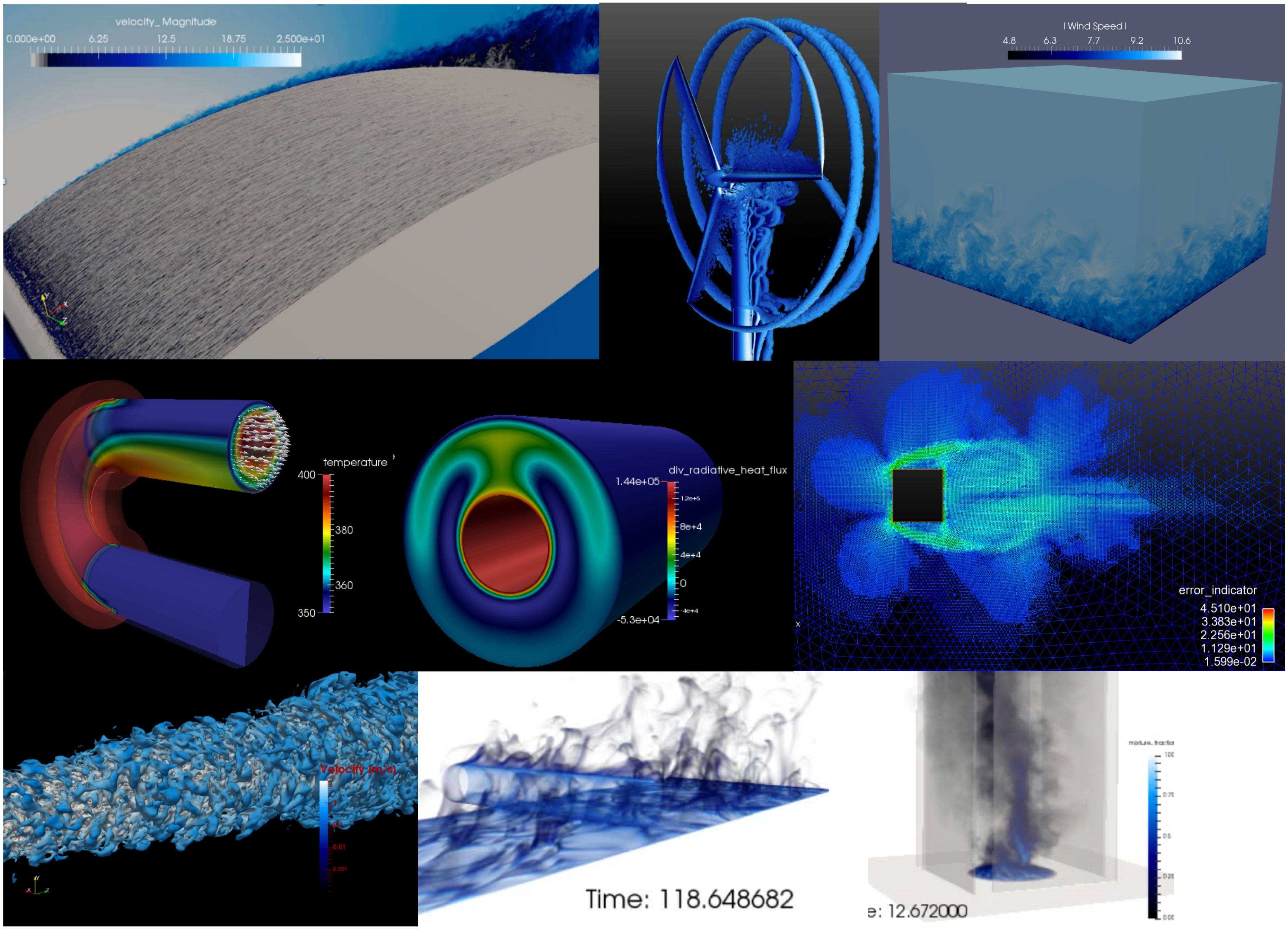
- Circa 2013, many scientific production codes were limited to 32-bit
- Therefore, maximum simulation size for entities, e.g., node, edge, face, element, etc., was ~2.2 billion
- Next Generation Platforms were advocated to overcome poor MPI scaling and power needs to support Exascale computing (10^{18} floating point operations/second)
  - Platform architectures are not yet known



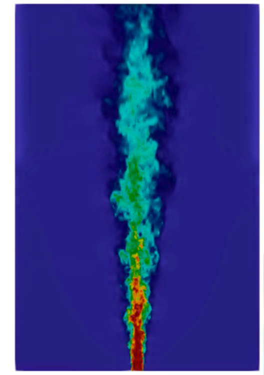
+ ASC IC Investments

Sierra Toolkit/Trilinos (open-source)
MPI+X parallelism
Support for new architectures

Supported Physics



Developed Open-Source BSD-clause 3 Distribution Policy



- Philosophy: Open-source collaborations

NALU LOW-MACH

https://github.com/NaluCFD

ASC™

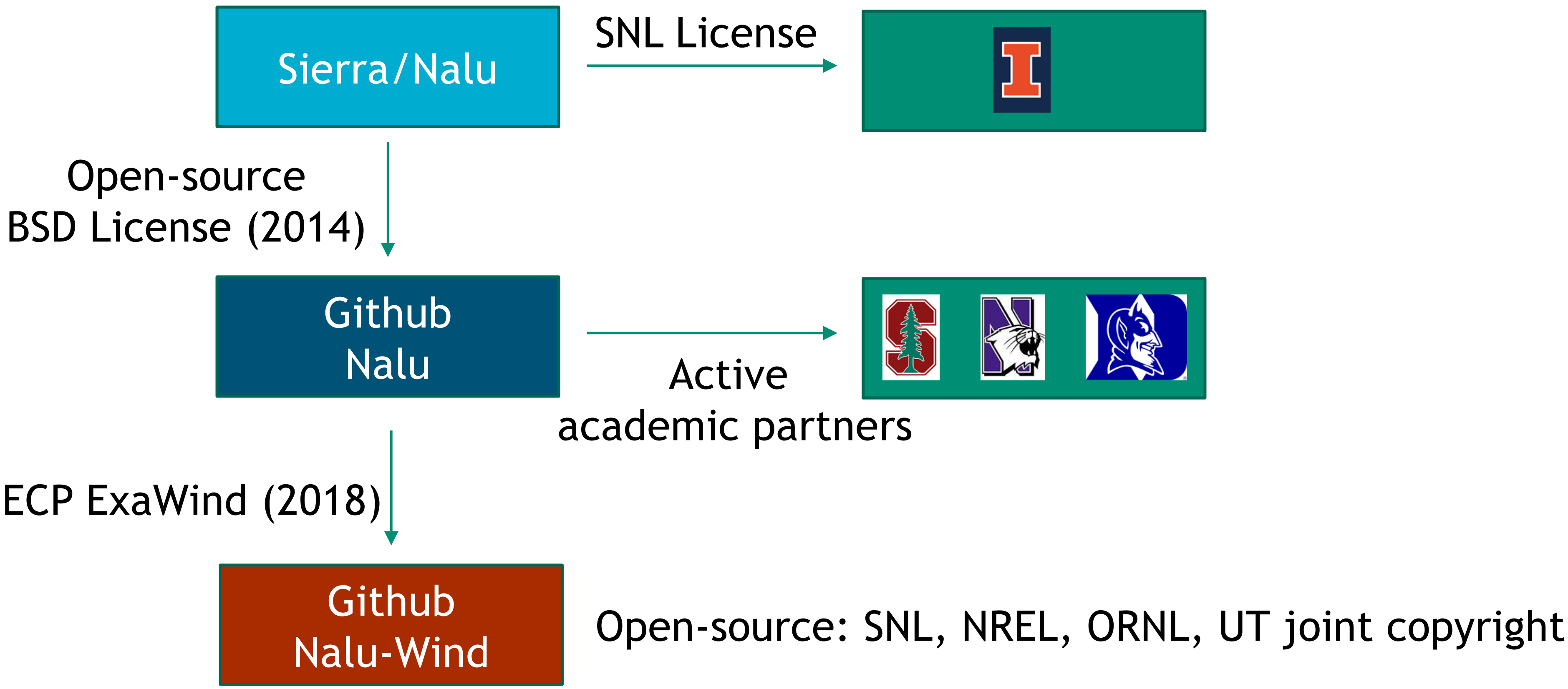
ECP EXASCALE COMPUTING PROJECT

ATMOSPHERE TO ELECTRONS
U.S. DEPARTMENT OF ENERGY

UPC (soon)

Nalu History

- A time-history of the Nalu code base:
- By CFD standards, this is a relatively new code base



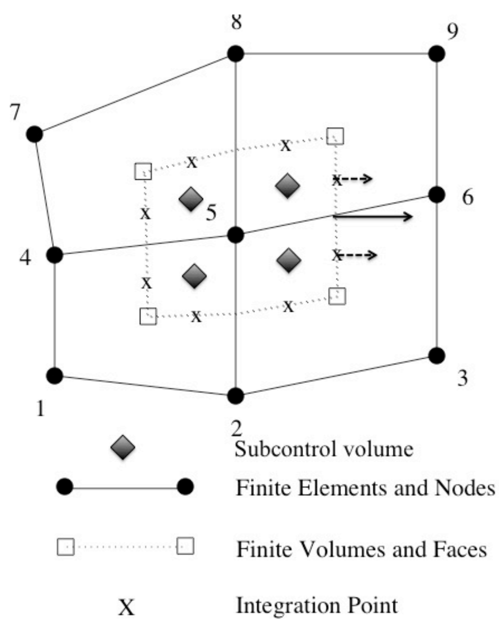
Supported Discretizations: CVFEM/FEM/EBVC

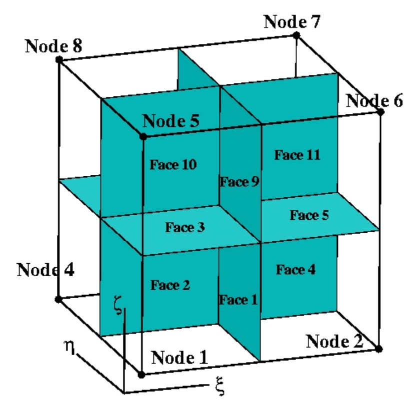
- The core discretization used in the low Mach code base has been the Control Volume Finite Element Method, CVFEM
- Finite Element Method and Edge-based Vertex-Centered, EBVC, are also supported

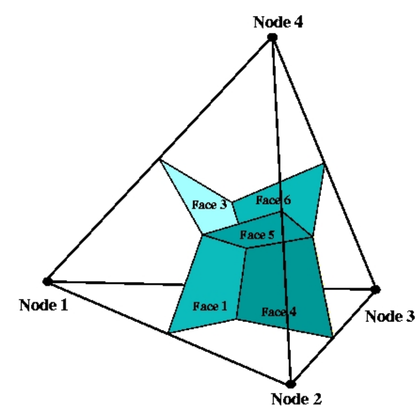
$$\int w \frac{\partial \bar{\rho} \tilde{u}_j \tilde{\phi}}{\partial x_j} d\Omega = -\int \bar{\rho} \tilde{u}_j \tilde{\phi} \frac{\partial w}{\partial x_j} d\Omega + \int w \bar{\rho} \tilde{u}_j \phi n_j \, d\Gamma$$

$$w = w_I ; \frac{\partial w_I}{\partial x_j} = -\delta(x - x_{scs})$$

$$\int w \frac{\partial \bar{\rho} \tilde{u}_j \tilde{\phi}}{\partial x_j} d\Omega = \sum_{ip} \left(\bar{\rho} \tilde{u}_j \right)_{ip} \tilde{\phi}_{ip} n_j dS = \sum_{ip} \dot{m}_{ip} \tilde{\phi}_{ip}$$

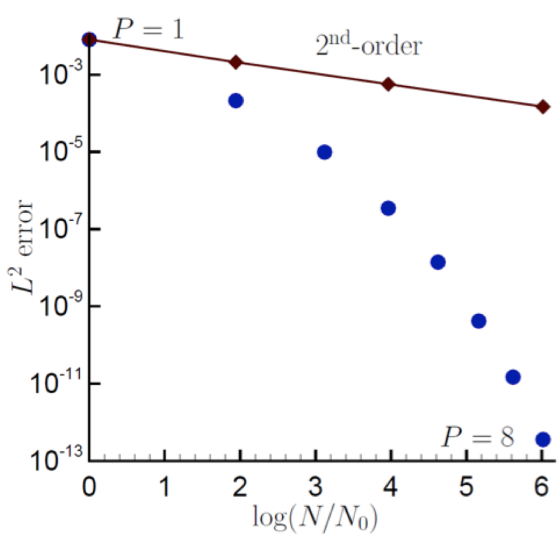




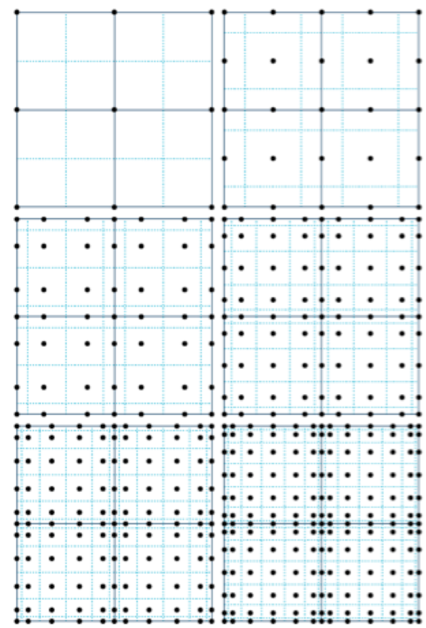


Scientific Research Platform to Evaluate Higher-Order Methods on Next Generation Platforms

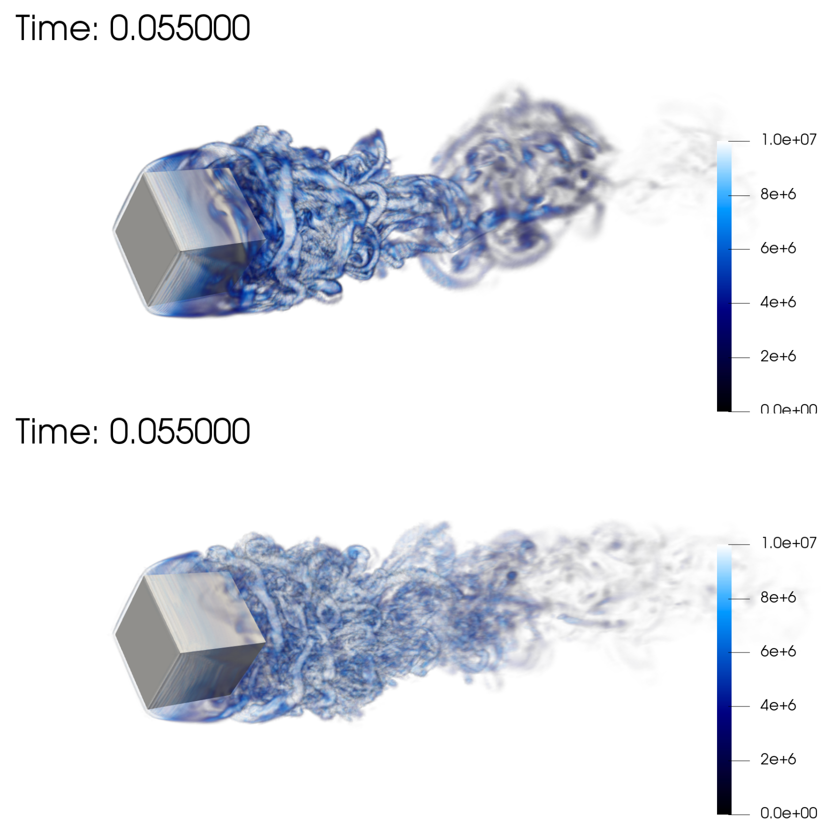
- As the cost of parallel assembly increases, should we strive to perform more local work? Higher-order achieves this design-point (at the cost of a larger memory footprint)



Spectral convergence



Dual-volume for promoted quad4

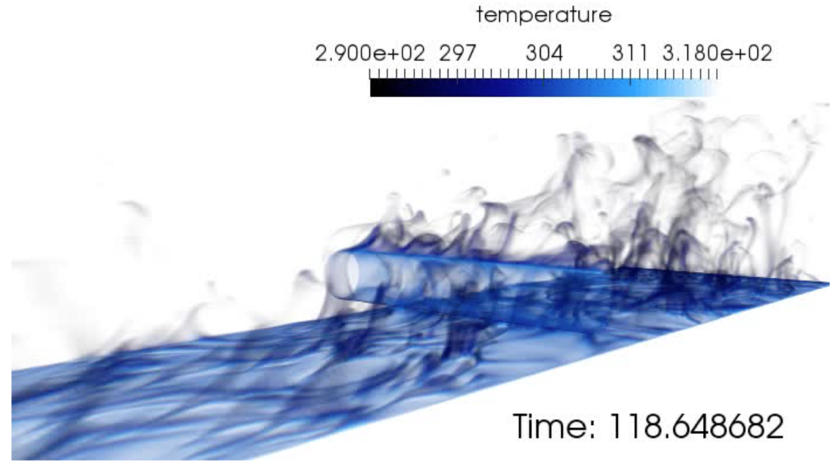


Flow-past rotating cube
Re~4000, RPM~3200
Same node count,
P=1 (top) P=2 (bot)

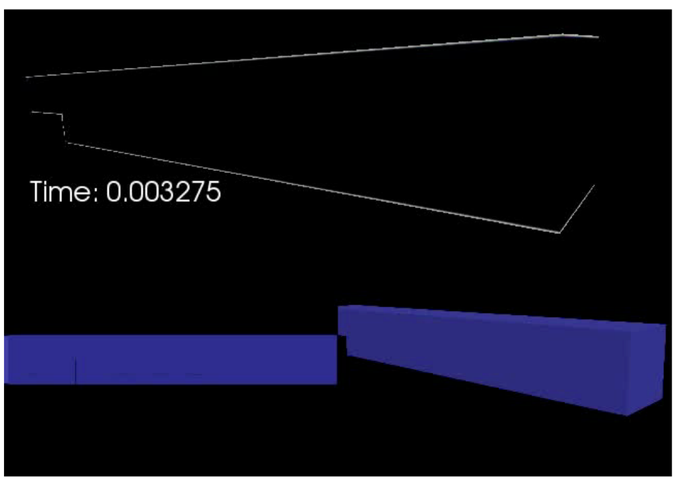
EXASCALE COMPUTING PROJECT

Several Multi-physics Flow Examples

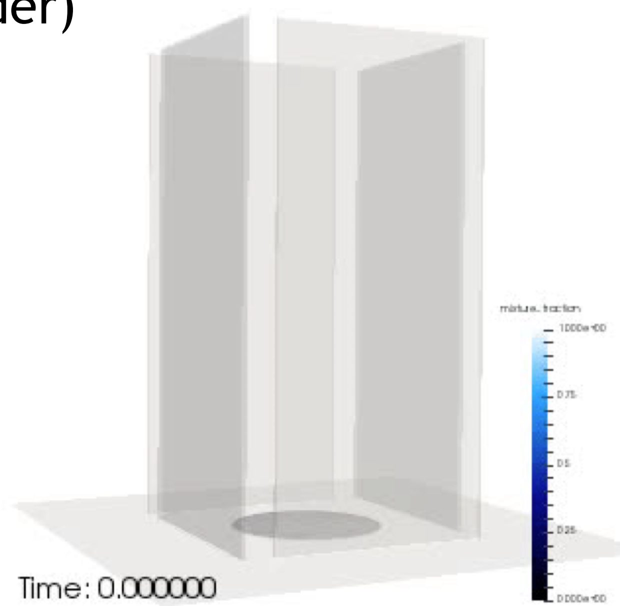
Helium plume (low-/high-order)



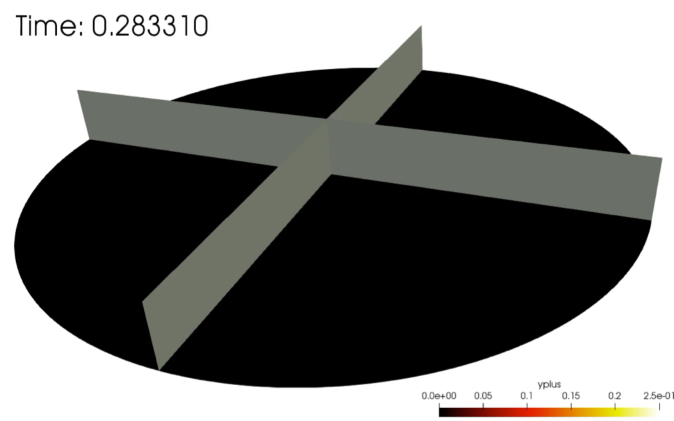
Cylinder in cross flow



Heated backstep



Whirling behavior

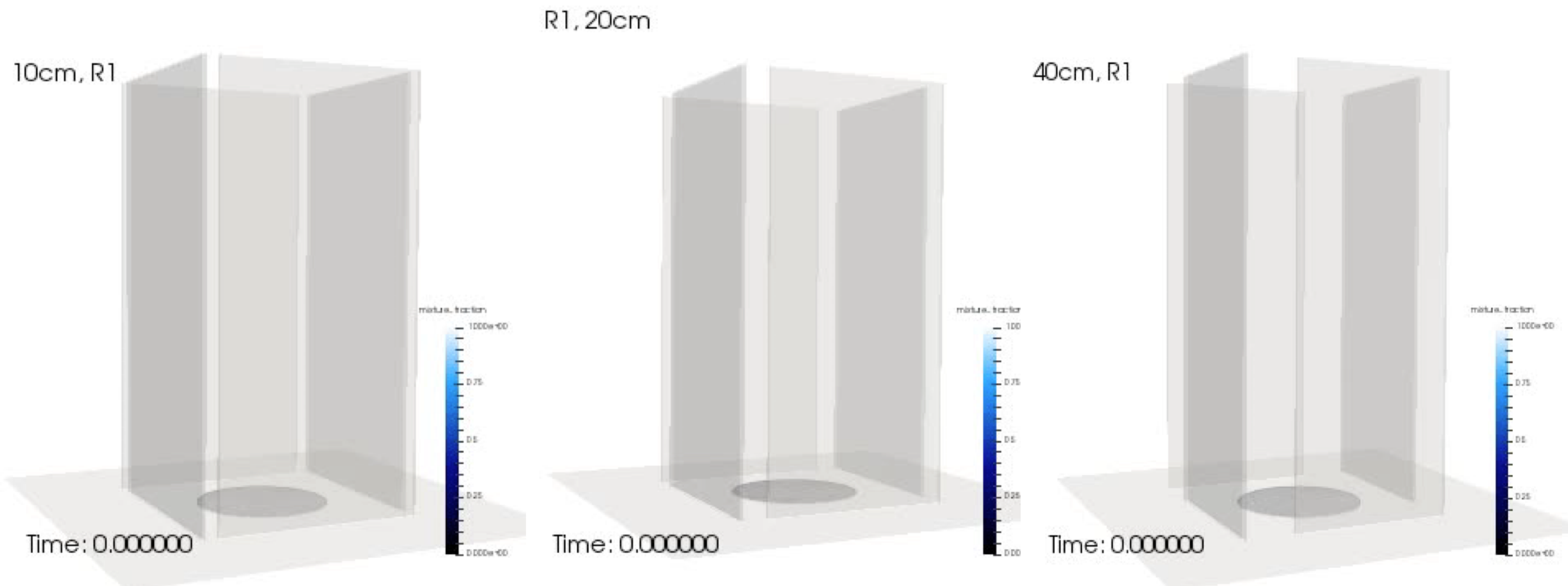


Impinging Jet DNS

Evolution of a Mindset….. Modeling Whirling-like Flow

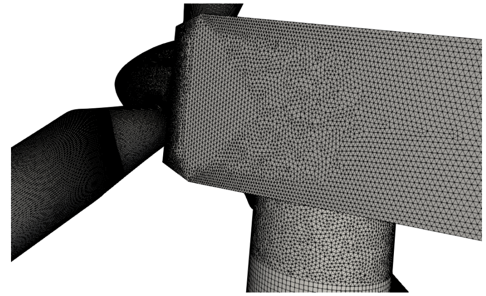
SAND2019-7052 C

- Idealized chamber in which swirl is provided by selective wall placement in the experimental design
- Gap varied between 10, 20, and 40 cm
- Objective: Can the onset of swirl be predicted? What is the strength?



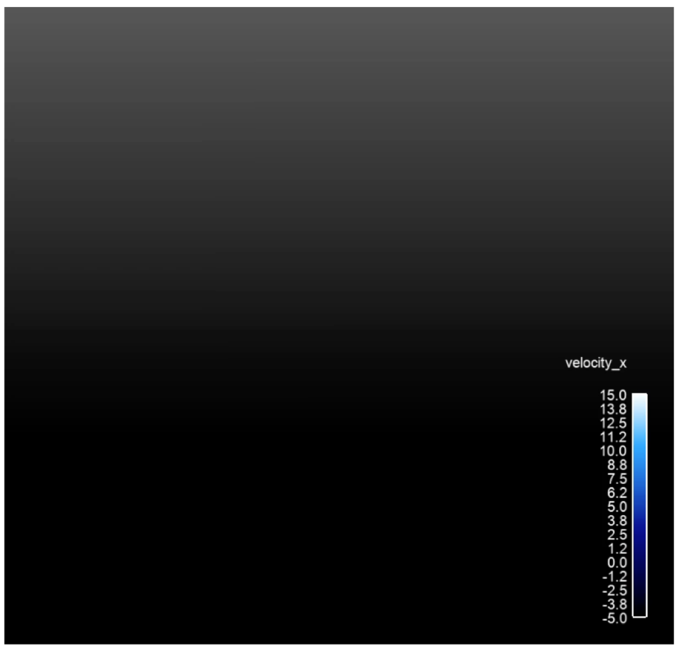
Volume rendered mixture fraction

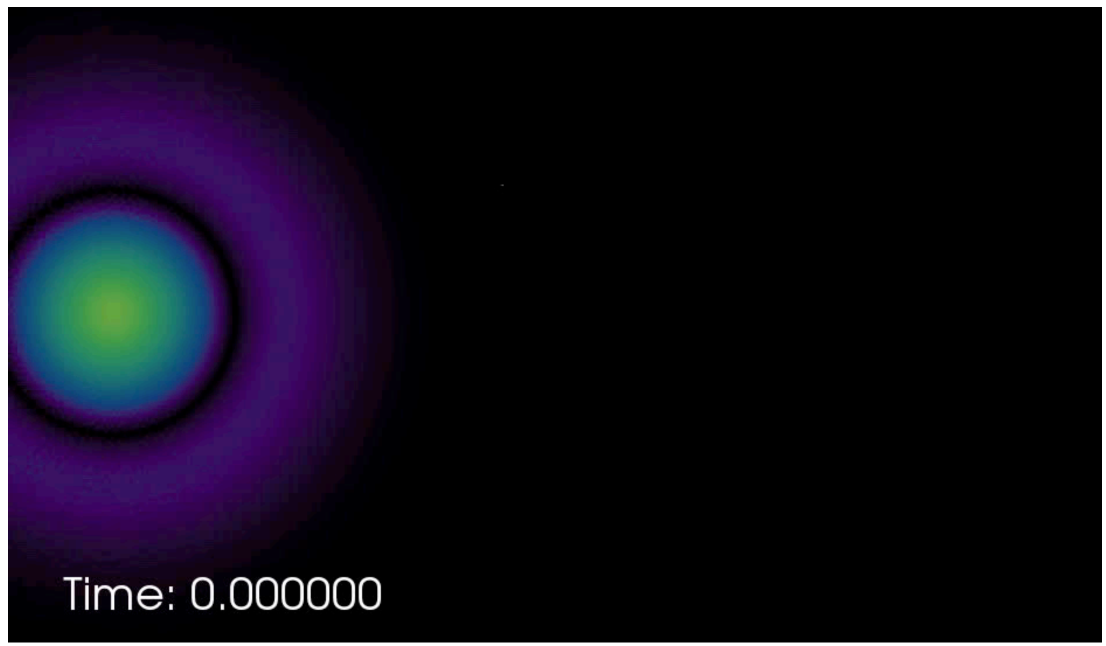
Unique Wind Energy Needs



- Low-dissipation methods with suitable nonlinear stabilization operators to perform blade-resolved physics
- Complex rotating blades, pitching blades, with possible yaw
- Transition from low-order (near the blade) to higher-order (in the wake)

Generalized, unstructured, hybrid low-order simulations shown

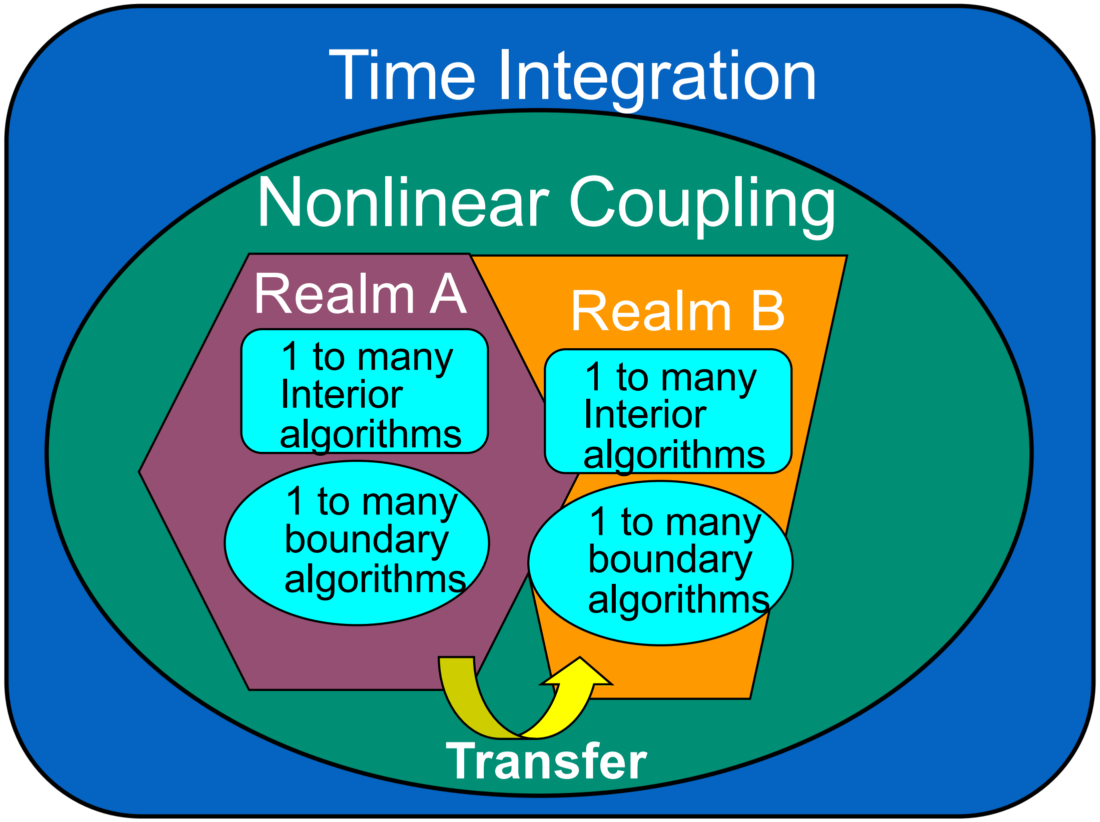




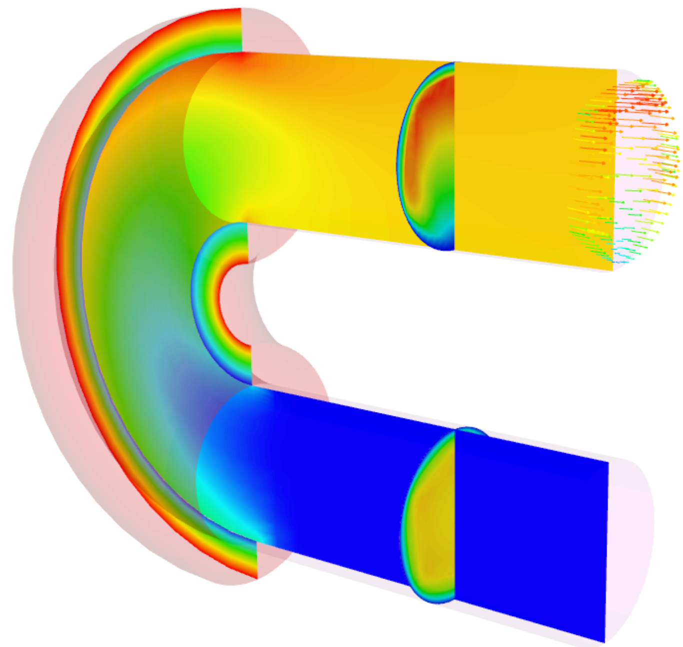
Horizontal Axis Wind Turbine (HAWT)

Vertical Axis Wind Turbine (VAWT)

Nalu Abstractions: Polymorphic and Input File-Driven



- *Realm* specifications define the physics and desired boundary conditions
- Pre-defined *EquationSystems* (segregated or monolithic)



Operator-split multi-physics
Conjugate heat transfer coupling

- Fluids Realm
- Heat Conduction Realm

30K View: Anatomy of a Nalu Input File:YAML-based

```
Simulation:

linear_solvers:

transfers:

realms:

  - name: realm_heatCond

    boundary_conditions:
    - wall_boundary_condition: bc_exposed

    solution_options:
    initial_conditions:
    material_properties:
    equation_systems:

      systems:
        - HeatConduction:

    output:
    restart:

  - name: realm_fluids

TimeIntegrators:
```

linear_solvers: Specification of sparse Trilinos-based precond/solver

transfers: Data transfer for multi-physics coupling

YAML enforces strict spacing and ordering

https://www.democraticunderground.com/10021540110

boundary_conditions: through restart: Physics definitions

TimeIntegrators: Time integration, e.g., BE, BDF2

High-Level Elements of an Input File

```
systems:

  - LowMachEOM:
      name: myLowMach

  - MixtureFraction:
      name: myZ
```

```
initial_conditions:

  - constant: ic_1
      target_name: [block_1, …]
      value:
        pressure: 0
        velocity: [0.5,0.0]
        mixture_fraction: 0.0
```

```
boundary_conditions:

  - inflow_boundary_condition: bc_left_inflow
  - wall_boundary_condition: bc_front_wall
  - open_boundary_condition: bc_right_open
  - symmetry_boundary_condition: bc_top
  - nonconformal_boundary_condition: bc_nc
```

```
material_properties:

 target_name: block_1

 specifications:

   - name: density
     type: constant
     value: 1.0

   - name: viscosity
     type: constant
     value: 1.8e-5
```

```
material_properties:

 target_name: block_1

 specifications:

   - name: density
     type: ideal_gas

   - name: viscosity
     type: polynomial
     coefficient_declaration:
```

```
 - inflow_boundary_condition: bc_left
     target_name: surface_1
     inflow_user_data:
       velocity: [0.5,0.0,0.0]
       mixture_fraction: 0.0

- wall_boundary_condition: bc_back
    target_name: surface_7
     wall_user_data:
       user_function_name:
        velocity: wind_energy
       user_function_string_parameters:
        velocity: [mmTop_ss7]
       mixture_fraction: 1.0
```

Test Case Input Files

- All input files are part of the Nalu regression test suite: Nalu/reg_test/test_files
- Mesh files are found under: Nalu/reg_test/mesh
  - Formally, /mesh is a git submodule

Test Cases Highlighted:

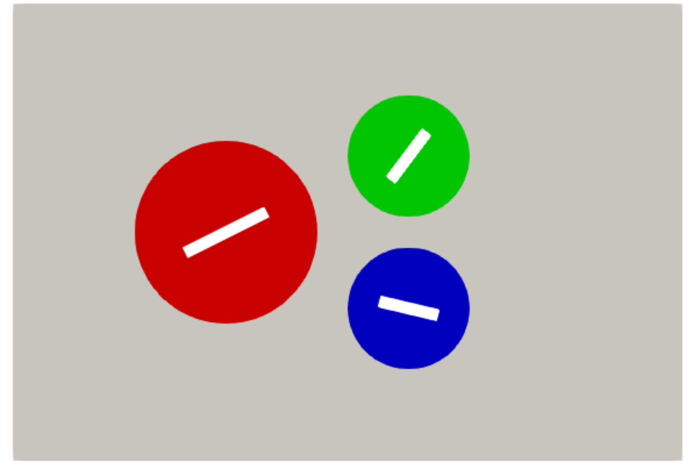
1. Nalu/reg_tests/test_files/dgNonConformalThreeBlade
2. Nalu/reg_tests/test_files/fluidsPmrChtPeriodic
3. Homework #1:
   1. https://github.com/spdomin/Present/tree/master/standformMe469/hwOne

- Feel free to run any case that you feel looks interesting to you!
- Note that the regression test suite is (mostly) focused on providing code coverage and may not represent "sane" physics-based choices

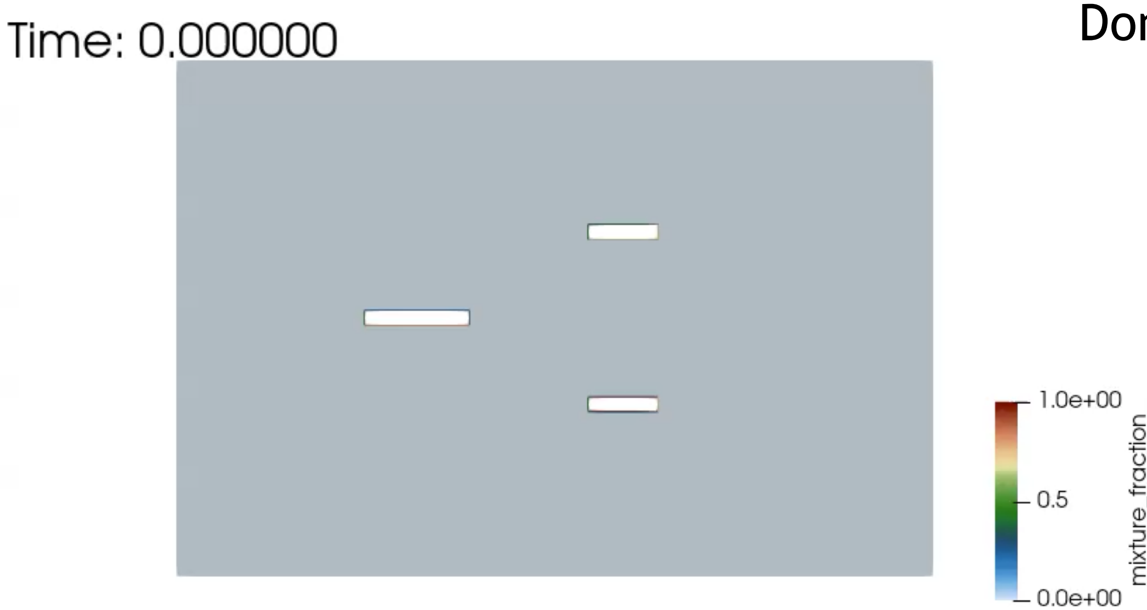
Resource: https://nalu.readthedocs.io/en/latest/source/theory/index.html

Nalu/reg_tests/test_files/dgNonConformalThreeBlade

- Physics
  - Flow past rotating square blades (Re = 10,000)
- Models
  - Newtonian fluid (air) with constant properties
- Boundary Conditions
  - Inflow, open, symmetry, DG/CVFEM interface



Domino, JCP, 2018



>mpirun --np 4 /naluPath/naluX -i dgNonConformalThreeBlade.i &

Nalu/reg_tests/test_files/dgNonConformalThreeBlade

$U\Delta t/\Delta x$

γ_i for BDF2

```
Time Step Count: 7 Current Time: 0.0127268
 dtN: 0.00266002 dtNm1: 0.00231306 gammas: 1.53488 -2.15 0.615116

Max Courant: 1.54421 Max Reynolds: 236.792 (realm_1)
   Realm Nonlinear Iteration: 1/1

realm_1::advance_time_step()
NLI      Name                Linear Iter       Linear Res       NLinear Res       Scaled NLR
---      ----                -----------       ----------       -----------       ----------
1/2      Equation System Iteration
 1/1        myLowMach
          MomentumEQS                  4       1.27653e-07      0.000173716                1
          ContinuityEQS                9       5.17721e-06       0.00618278                1
          PNGradPEQS                  19        4.2818e-09      2.78318e-06                1
          PNGradUEQS                  20       9.70201e-09      5.20951e-06                1
 1/1                myZ
          MixtureFractionEQS           5       1.31346e-09      6.84724e-06                1
          PNGradZEQS                   5       6.33586e-09      3.66957e-06                1
2/2      Equation System Iteration
 1/1        myLowMach
          MomentumEQS                  5       8.33682e-10      2.23818e-06        0.0128842

Mass Balance Review:
Density accumulation: 0
Integrated inflow:    -0.375
Integrated open:      0.3749998354138842
Total mass closure:   -1.64586e-07
Mean System Norm: 0.0002458198407611864 7 0.0127268
```

$\rho U L / \mu$

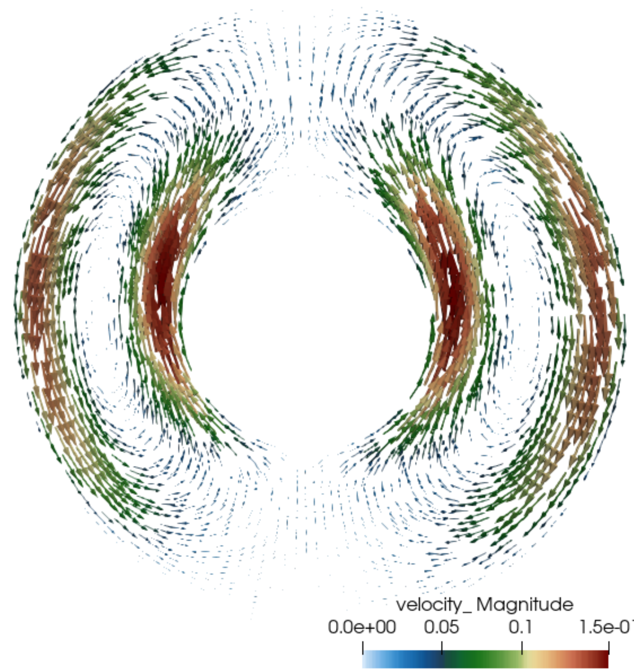
equations

nonlinear iterations

Review

Nalu/reg_tests/test_files/fluidsPmrChtPeriodic

- Physics
  - Uniformly emitting/absorbing participating media radiation (PMR) conjugate heat transfer (CHT) with buoyancy
- Models
  - Newtonian fluid (air): ideal gas
- Boundary Conditions
  - Wall, periodic

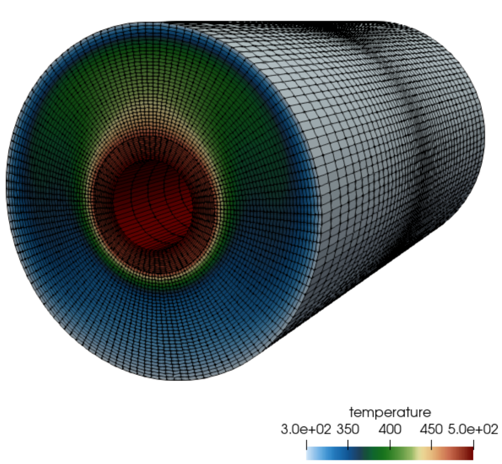


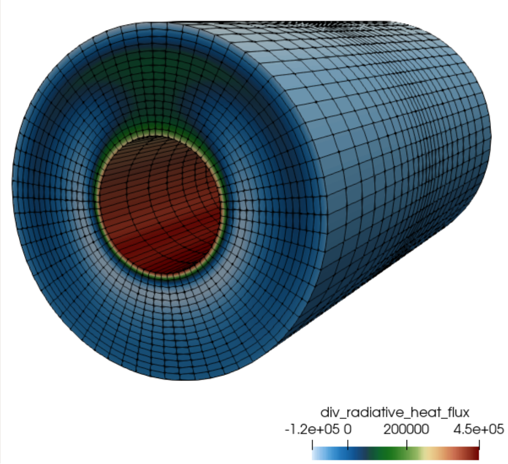
Stark#, cond/rad

$Sk = \lambda\ \mu\ /\ \sigma\ T_i^3 \sim 0.4$

Rayleigh#, $\tau^{ThermalDiff} / \tau^{Conv}$

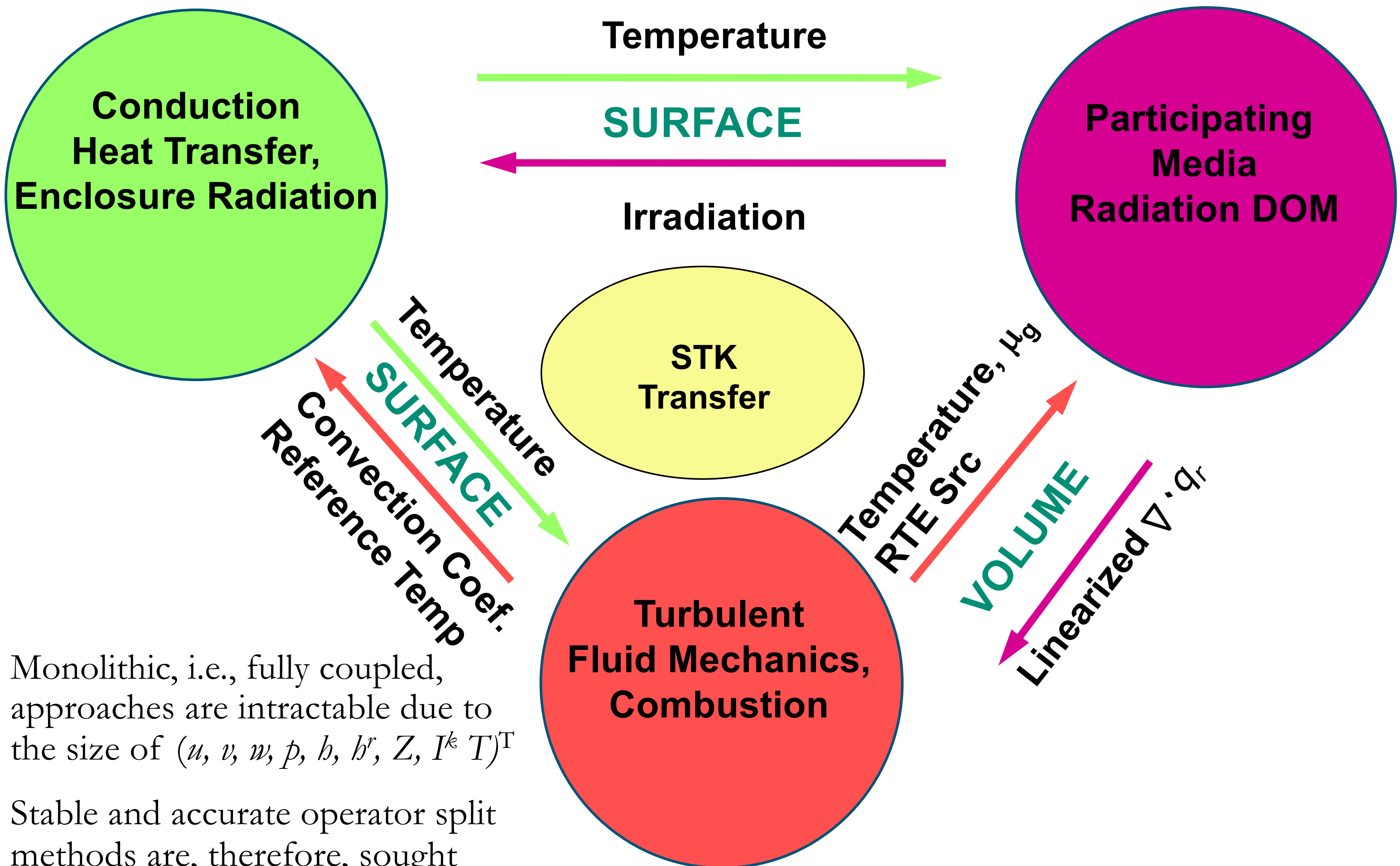
$Ra = g\ \beta\ (T_i - T_o)\ L\ /\ Pr\ \alpha^2 \sim 2e6$






```
>mpirun --np 8 /naluPath/naluX -i fluidsPmrChtPeriodic.i &
```

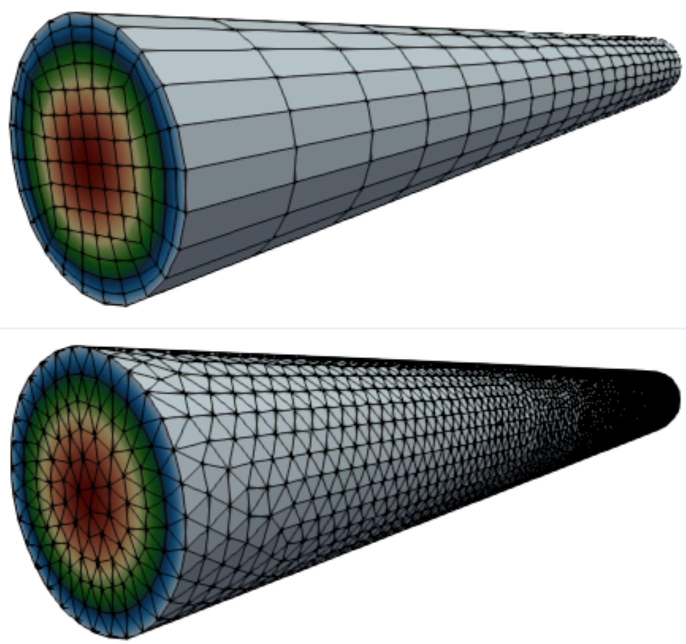
Nalu/reg_tests/test_files/fluidsPmrChtPeriodic



- Monolithic, i.e., fully coupled, approaches are intractable due to the size of $(u, v, w, p, h, h^r, Z, I^k\ T)^T$
- Stable and accurate operator split methods are, therefore, sought
  - See Domino et al., *AIAA*, 2007

- Physics
  - Laminar pipe flow (specified pressure drop)
- Models
  - Newtonian fluid (air): ideal gas
- Boundary Conditions
  - Wall, open (pressure specified)
- Location:

  https://github.com/spdomin/Present/tree/master/stanfordMe469/hw/one
- Specifications:
  - $Re^{\tau} = 10$
  - Pipe diameter, $D = 0.01$ m
  - Pipe Length, $L = 0.2$ m
  - ρ = TBD
  - μ = TBD
  - dp/dz = TBD
  - Uc = TBD



Nalu Overview: Conclusion

- Nalu's technology has its roots in the ASC Sierra/Fuego effort
- Multi-physics capabilities are in development
- Research platform for high-order low-Mach methods
- Open-source collaboration model
- Funded through ASC, ECP, A2e, ASCR, and LDRD