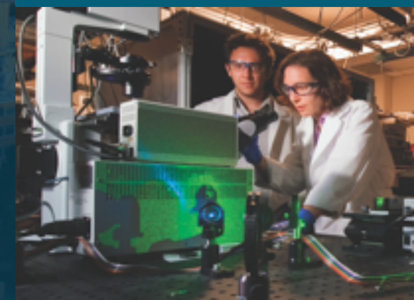
# Stanford ME469: Nalu Overview




PRESENTED BY

Stefan P. Domino

Computational Thermal and Fluid Mechanics

Sandia National Laboratories SAND2018-4619 PE



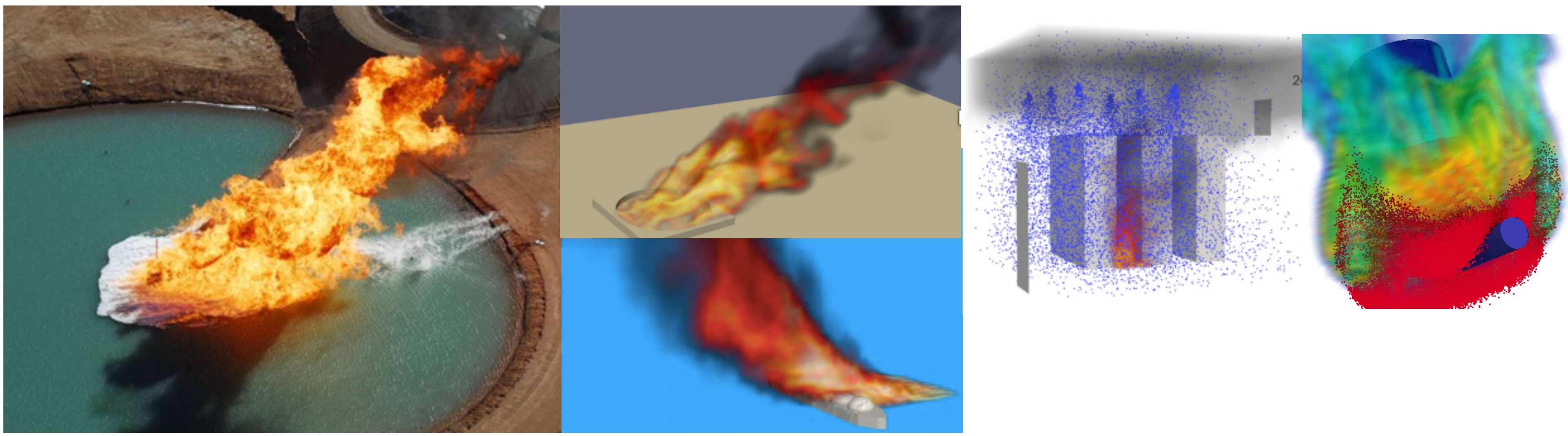
Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

# 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

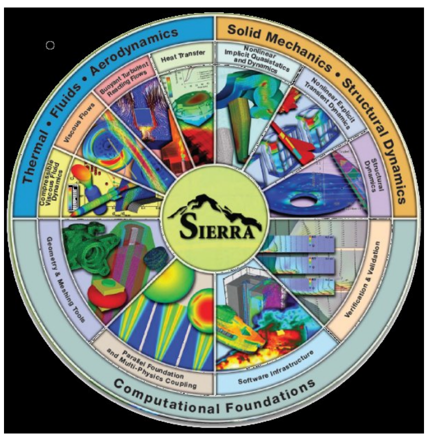
- Use-case characterized by a highly sooting, turbulent, reacting flow with Participating Media Radiation (PMR), Conjugate Heat Transfer (CHT), and propellant multi-physics coupling



- 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, at that point, were not not yet known (still evolving)





+ ASC IC Investments

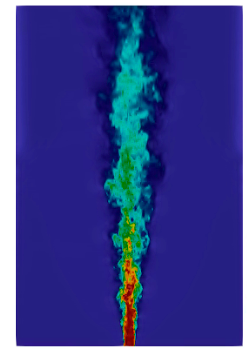
(  )

Sierra Toolkit/Trilinos (open-source)

MPI+X parallelism

Support for new architectures

# Developed Open-Source BSD-clause 3 Distribution Policy

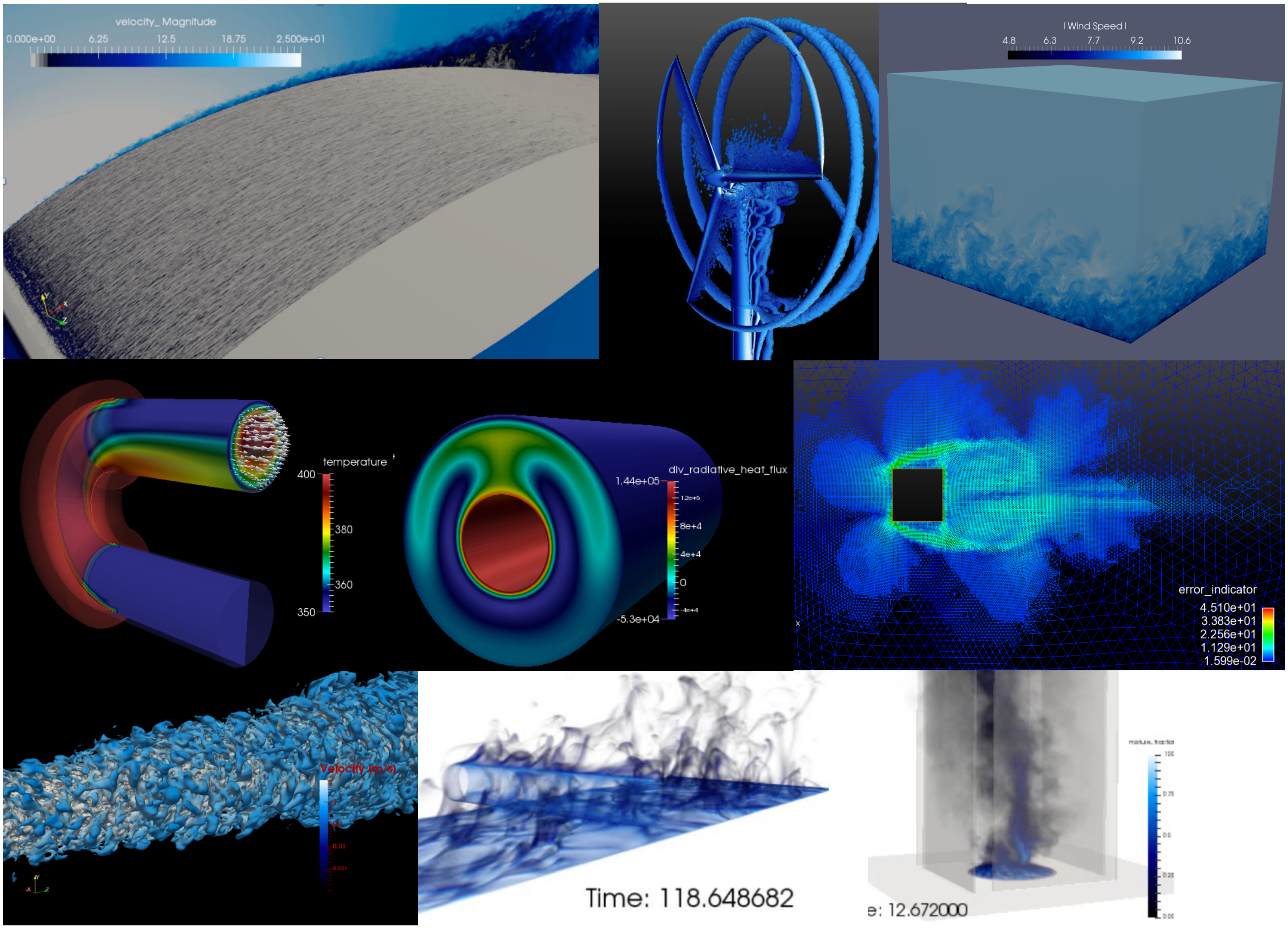


- Philosophy: Open-source collaborations

https://github.com/NaluCFD

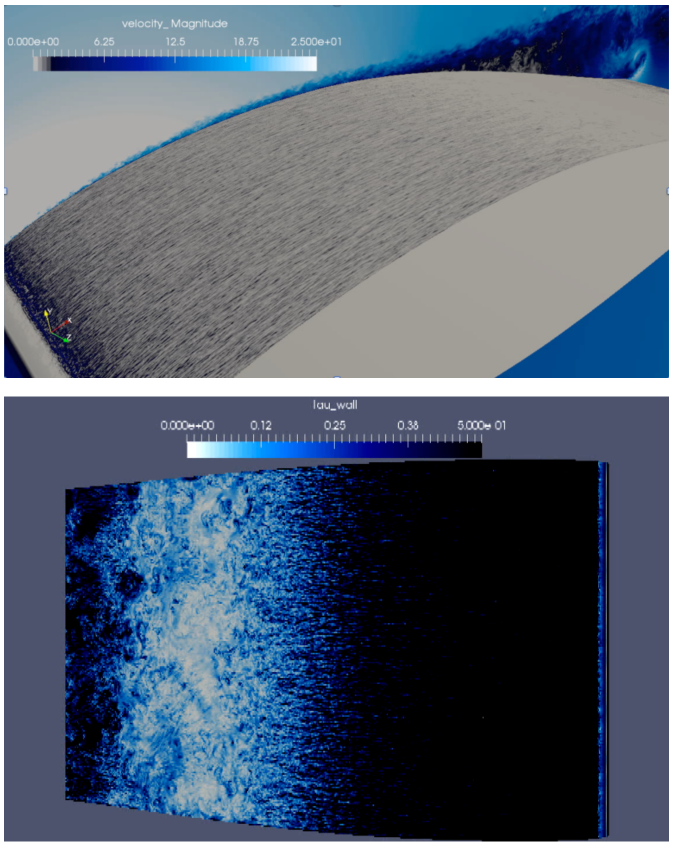
(soon)

# Supported Physics: DNS and LES (even RANS)

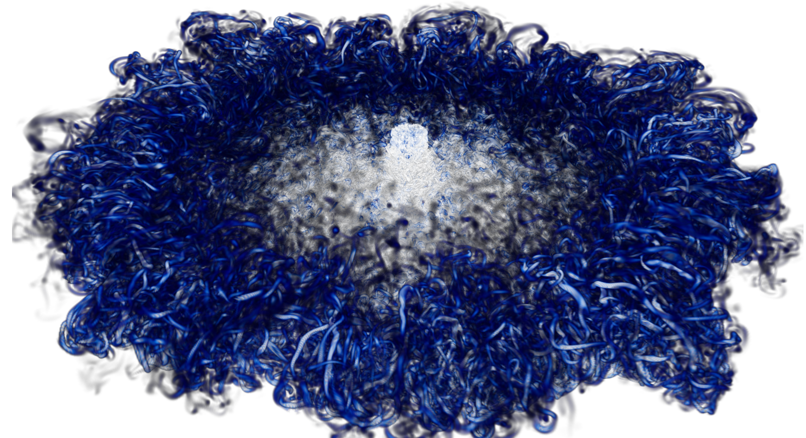


# A Note on High Performance Computing

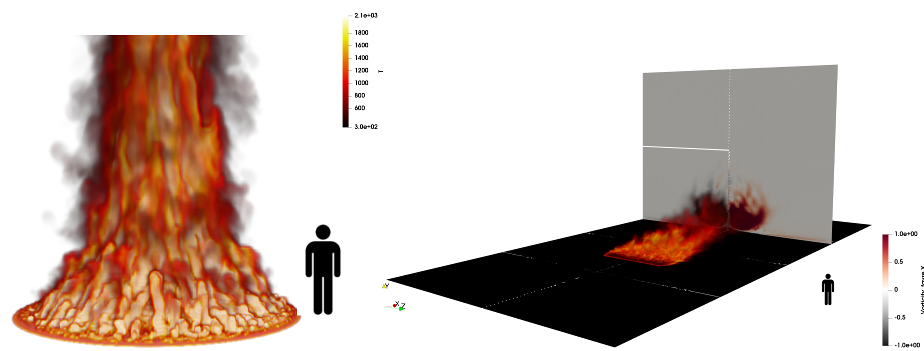
- Sandia is committed to High Performance Computing (HPC) to support is science and engineering objectives: Exercised herein




O(6) billion wind energy application



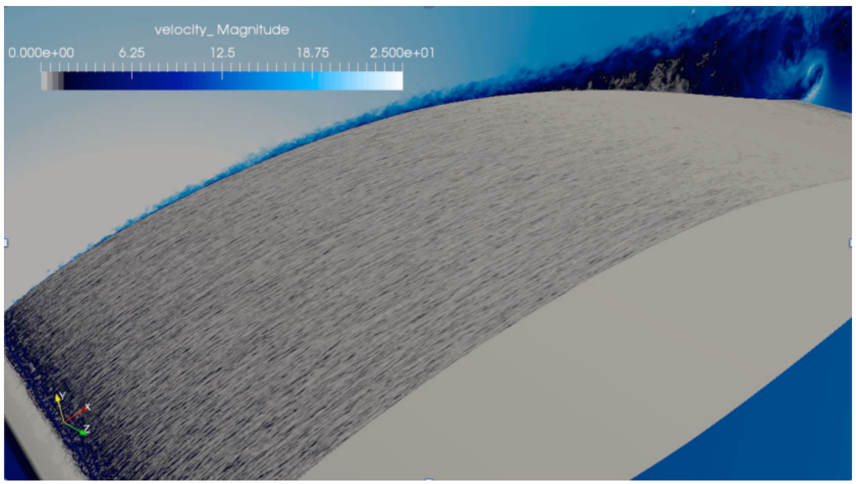
O(2) billion DNS impinging jet

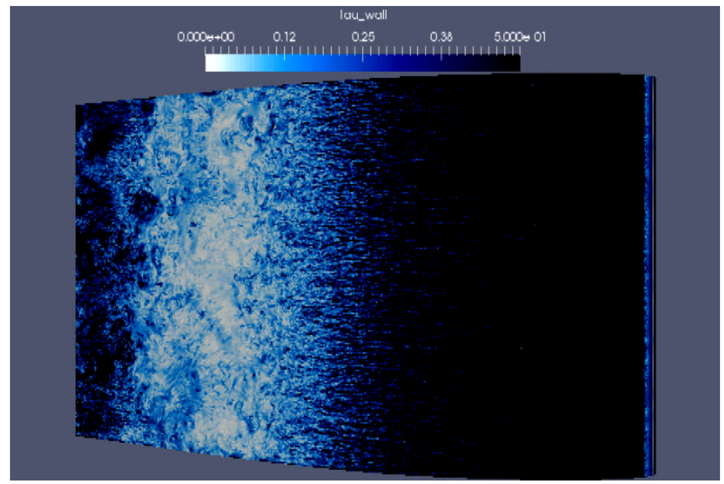


O(200) million multi-physics fire

# High Performance Computing: Working in Parallel

**Late Roman Timeline**
**250 AD - 300 AD**
250 AD: The Goths invade Anatolia (AKA, Asia Minor), in sea-borne raids they plunder *Nikopolis*

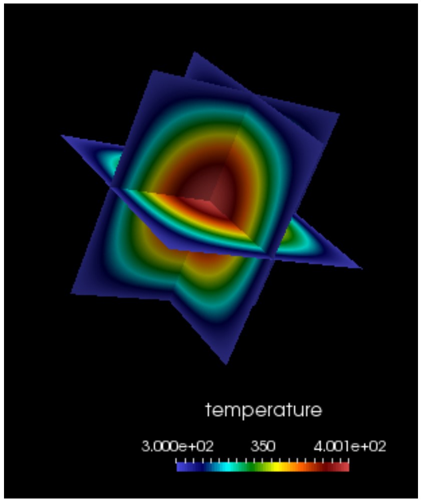


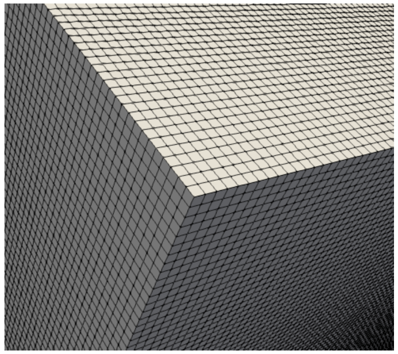



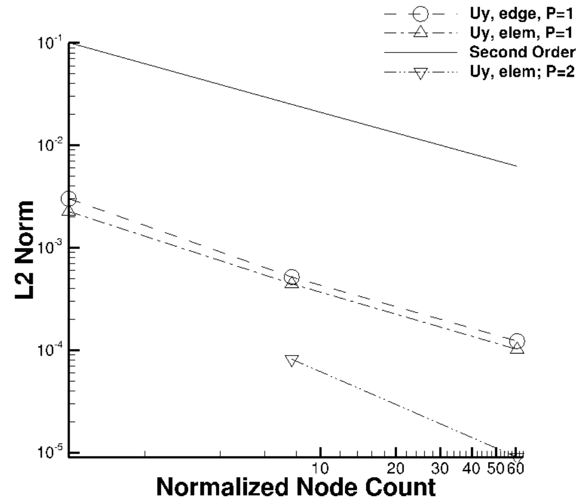

- Trinity open-science time, Domino and Barone, 2016 SAND2016-4085C to elucidate stall cells
- O(6) billion element wind energy application (high-Re flow past thick blade in high AoA
- O(128,0000) core run for ~one week ~1800 year simulation using computing resources available 10-years ago: Complete in roughly 29 years!

# Change of Philosophy: Former Approach

- Verify on ***nice*** Hexahedral-based elements

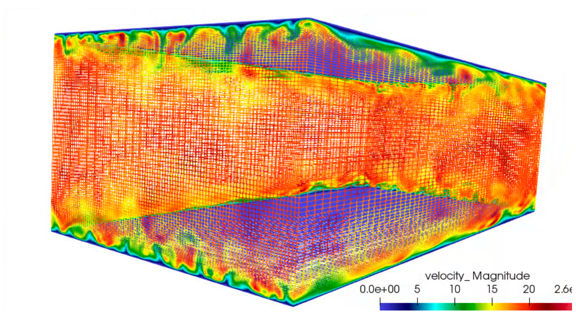


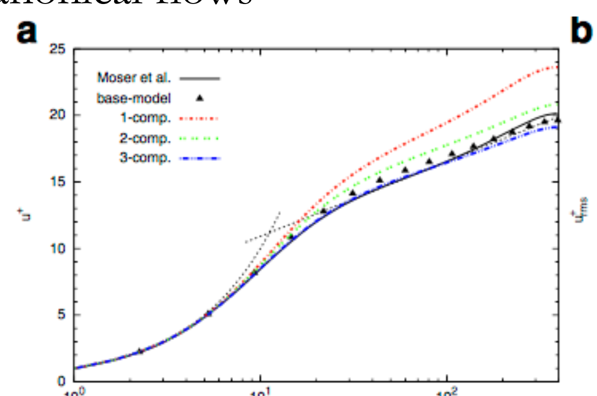






Variable-density low-Mach MMS (Domino, *CTRSP*, 2016)

- Validate on ***perfect*** meshes on a variety of canonical flows

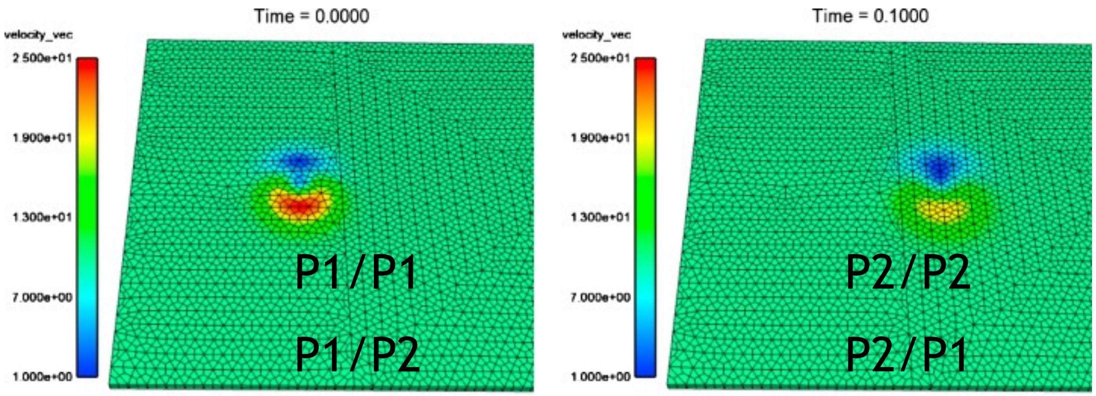



$Re_\tau$ 395 plane-channel (Jofre, Domino, Iaccarino, *Flow, Turb. & Comb.*, 2018)

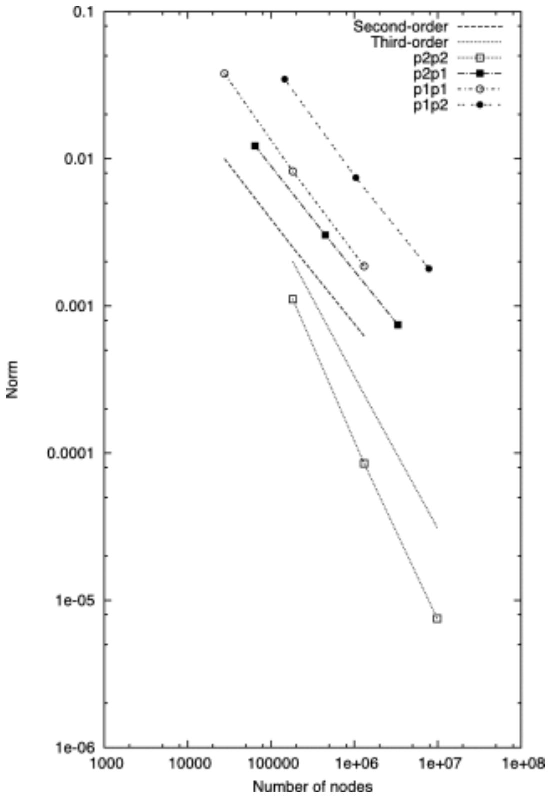
# Paradigm Shift: Verify and Deploy High-Quality Unstructured Numerical Methods

- Verify on ***awful*** hybrid mesh element quality

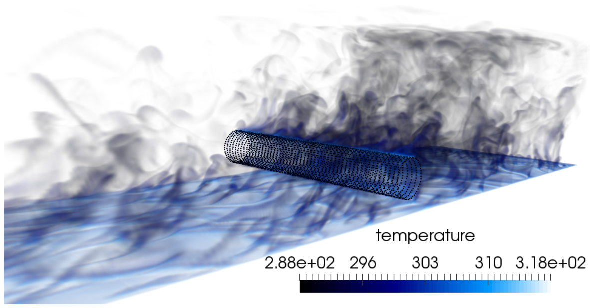



(a) Time = 0.0 seconds.

(b) Time = 0.10 seconds.



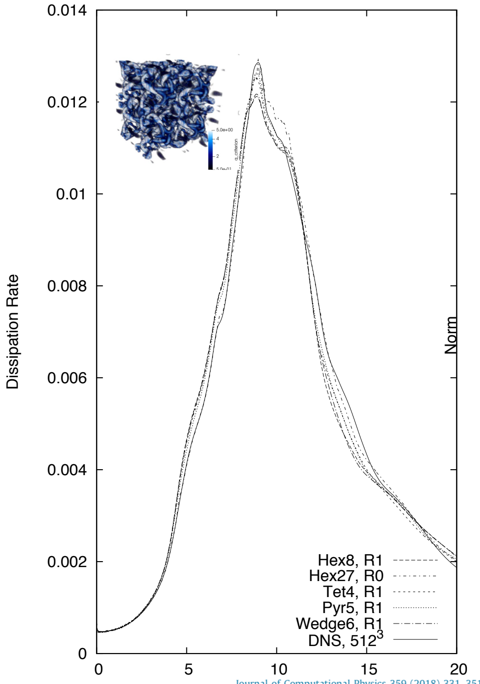

- Validate on ***non-ideal*** meshes on a variety of canonical flows

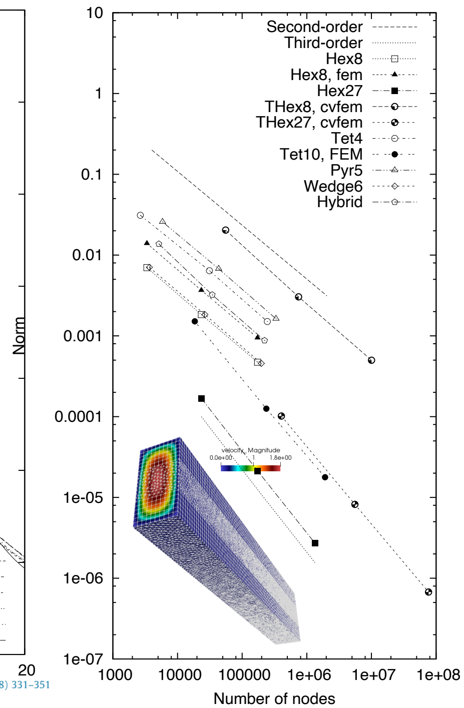



Domino, J. Comp. Phys. *Flow, 2018*

# Confidence Established for Atypical Element Topos

## Verification




Journal of Computational Physics 359 (2018) 331–351

Contents lists available at ScienceDirect

Journal of Computational Physics

ELSEVIER

Computers and Fluids 179 (2019) 655–669

Contents lists available at ScienceDirect

Computers and Fluids

journal homepage: www.elsevier.com/locate/compfluid

ELSEVIER

Design-
a hybri

Stefan P. 

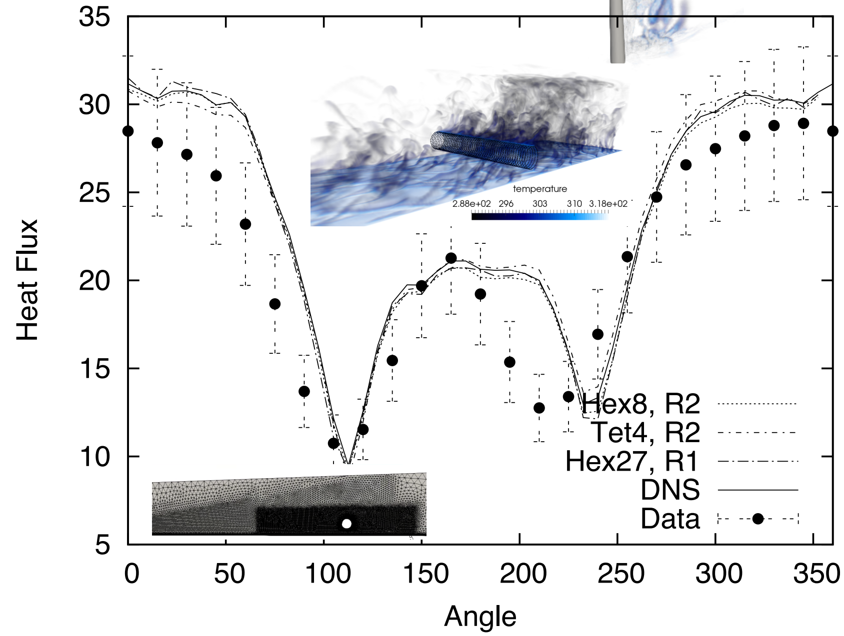
Sandia National
United States

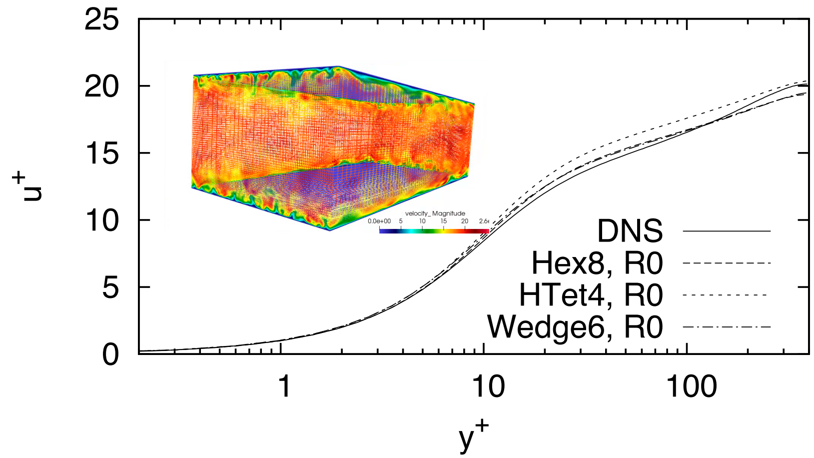
An assessment of atypical mesh topologies for low-Mach large-eddy simulation

Stefan P. Domino[a,b,*], Philip Sakievich[a,b], Matthew Barone[a,c]

[a] Sandia National Laboratories, P.O. Box 5800, Albuquerque, NM 87109, USA
[b] Computational Thermal and Fluid Mechanics Department, 1541, USA
[c] Aerosciences Department, 1515, USA

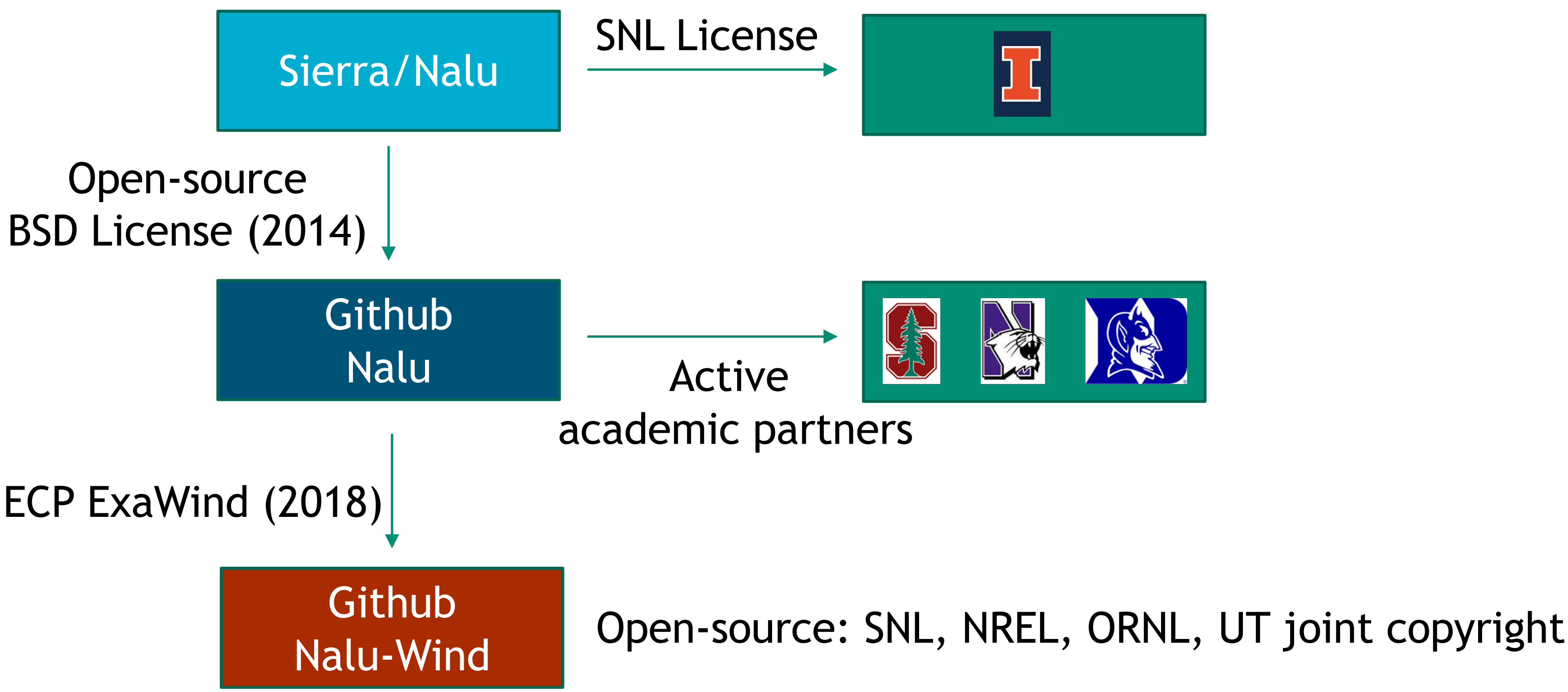
## Validation



# Nalu History

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



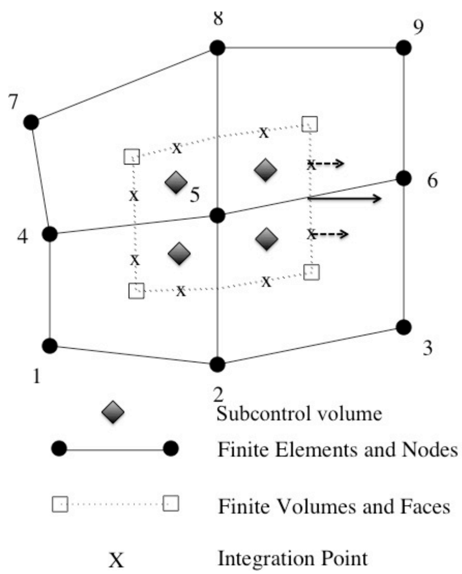
# Supported Discretizations: CVFEM/FEM/EBVC

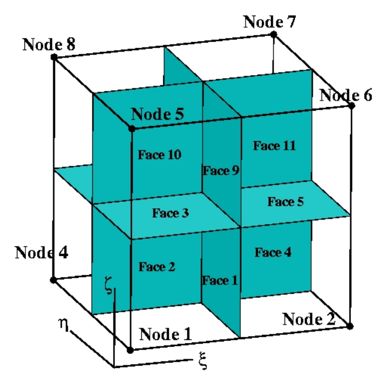
- The core discretization used in the low Mach code base has been the Control Volume Finite Element Method, CVFEM
- Finite Element Method and Edge-based Vertex-Centered, EBVC, are also supported

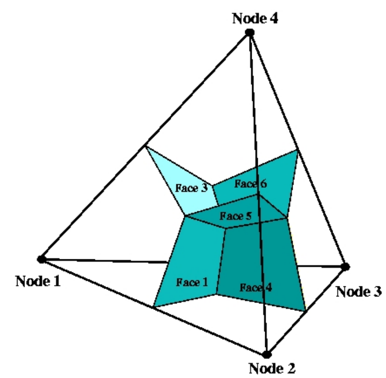
$$\int w \frac{\partial \bar{\rho} \tilde{u}_j \tilde{\phi}}{\partial x_j} d\Omega = -\int \bar{\rho} \tilde{u}_j \tilde{\phi} \frac{\partial w}{\partial x_j} d\Omega + \int w \bar{\rho} \tilde{u}_j \phi n_j \, d\Gamma$$

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

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

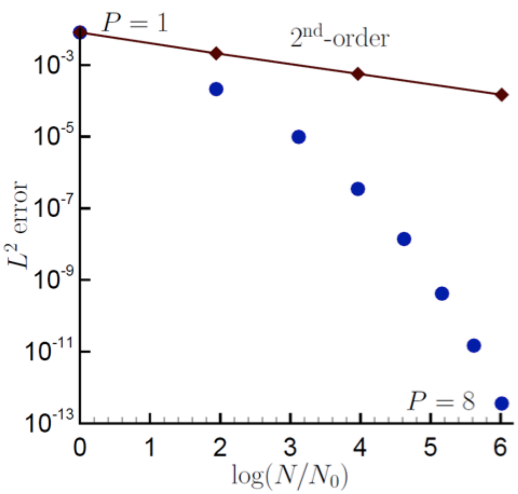


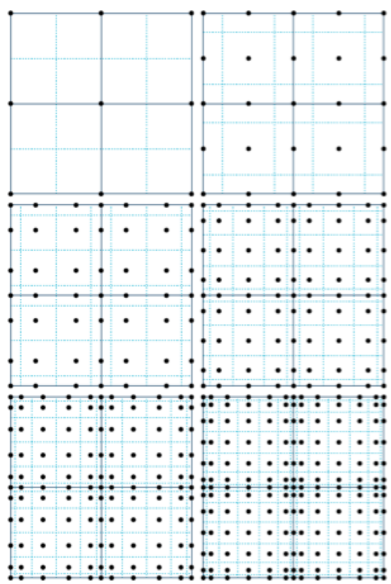



# Scientific Research Platform to Evaluate Higher-Order Methods on Next Generation Platforms

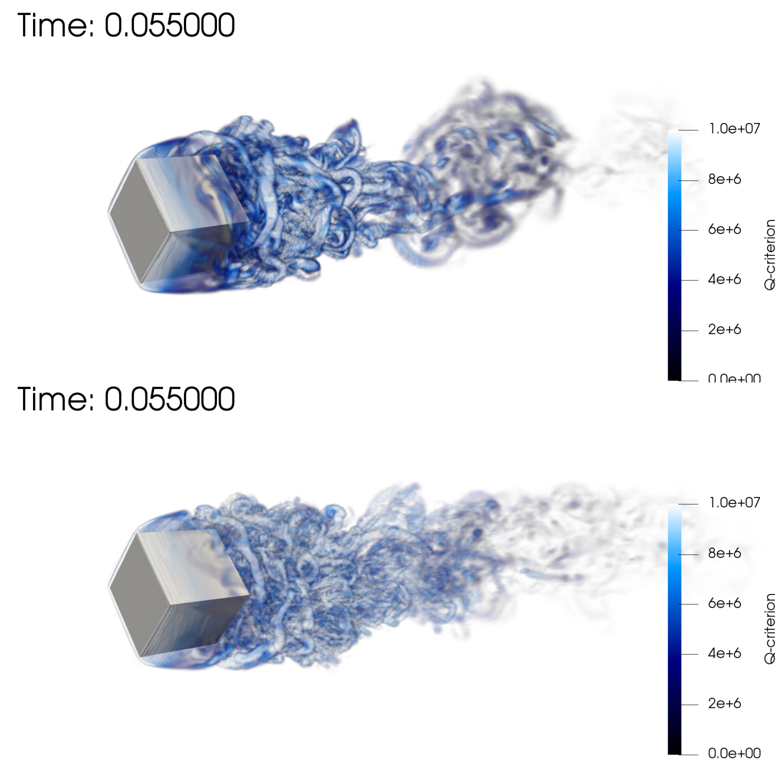
- As the cost of parallel assembly increases, should we strive to perform more local work? Higher-order achieves this design-point (at the cost of a larger memory footprint)




Spectral convergence



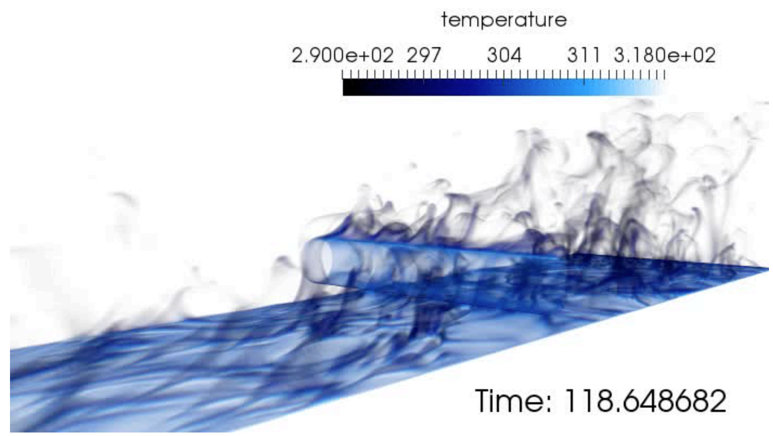
Dual-volume
for promoted quad4



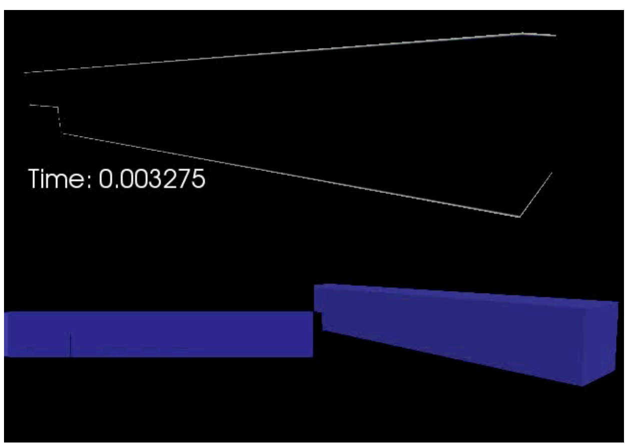

Flow-past rotating cube
Re~4000, RPM~3200
Same node count,
P=1 (top) P=2 (bot)

# Several Multi-physics Flow Examples From Nalu

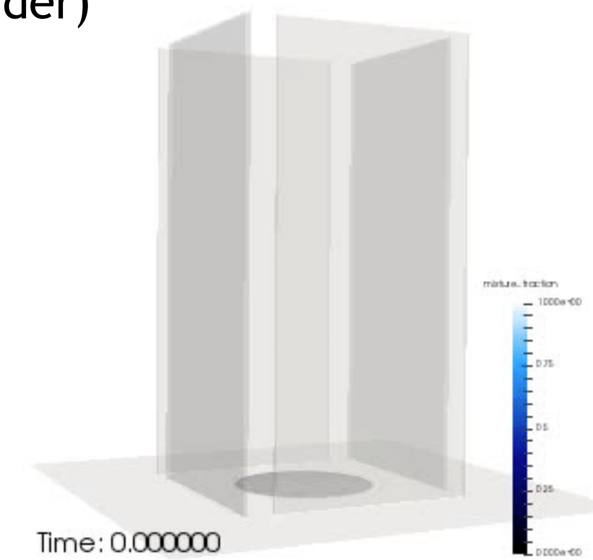

Helium plume (low-/high-order)



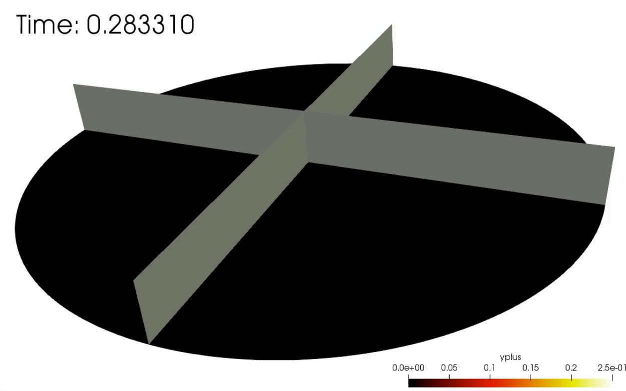

Cylinder in cross flow




Heated backstep




Whirling behavior

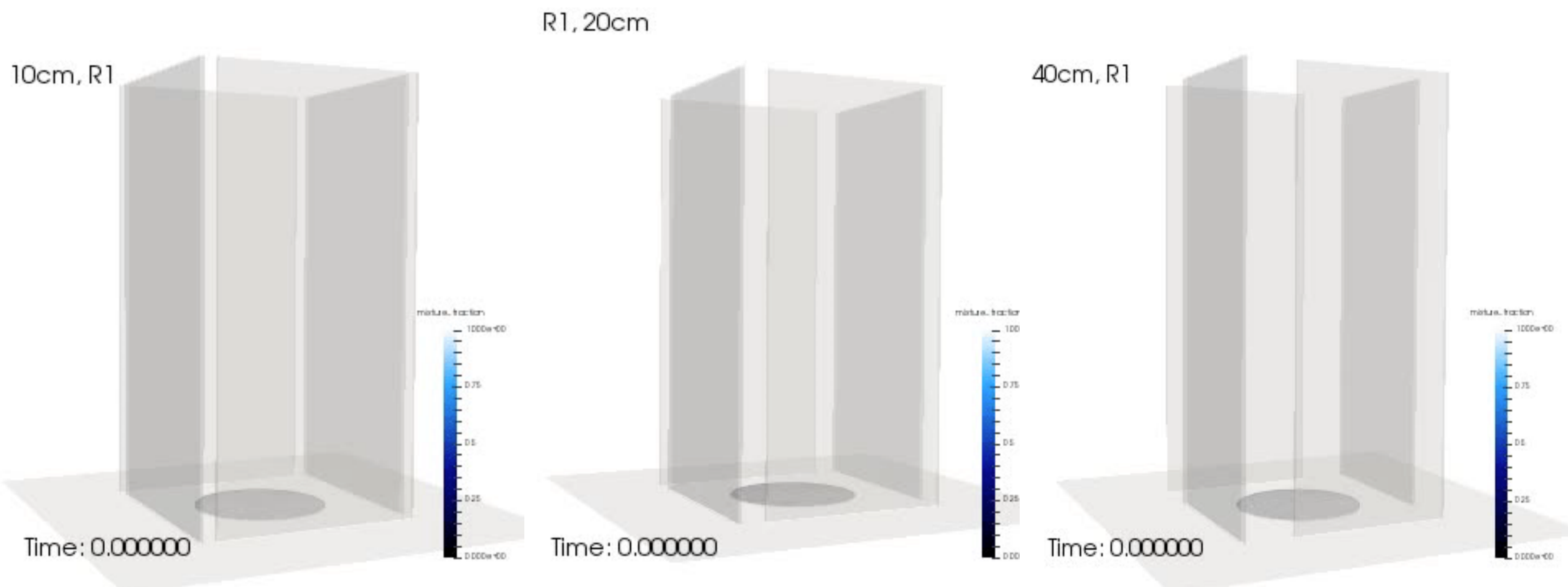



Impinging Jet DNS

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

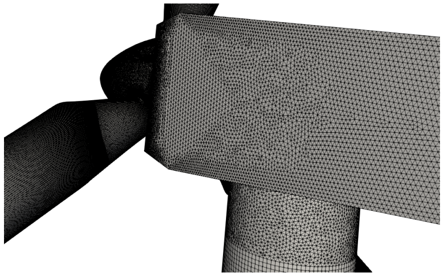
SAND2019-7052 C

- 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?

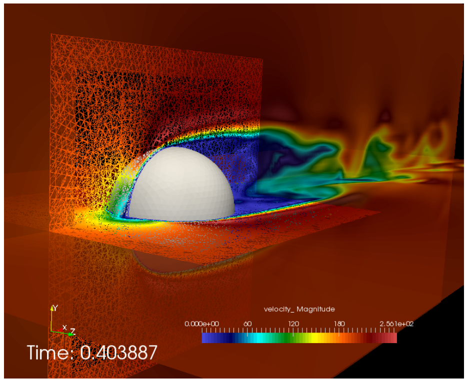


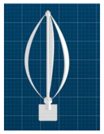

Volume rendered mixture fraction

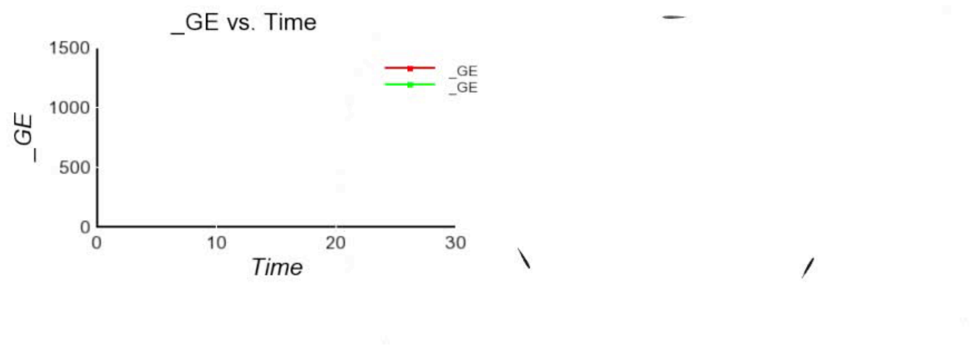
# Unique Complex Geometry Use-Cases

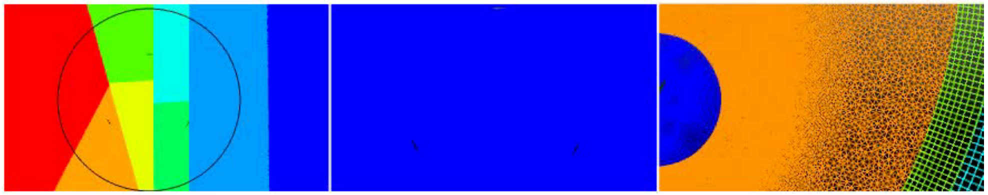


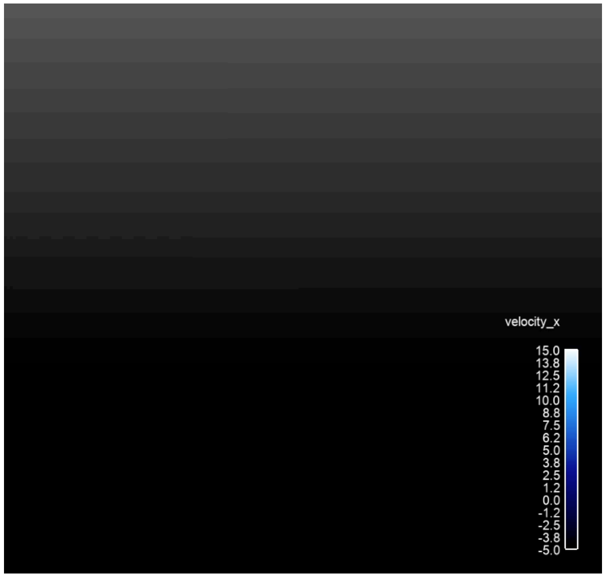
- Low-dissipation methods with suitable nonlinear stabilization operators using sliding and overset technologies to aid modeling effort and/or meshing
- Objective: Design-order established/verified implementations on generalized, unstructured, hybrid meshes





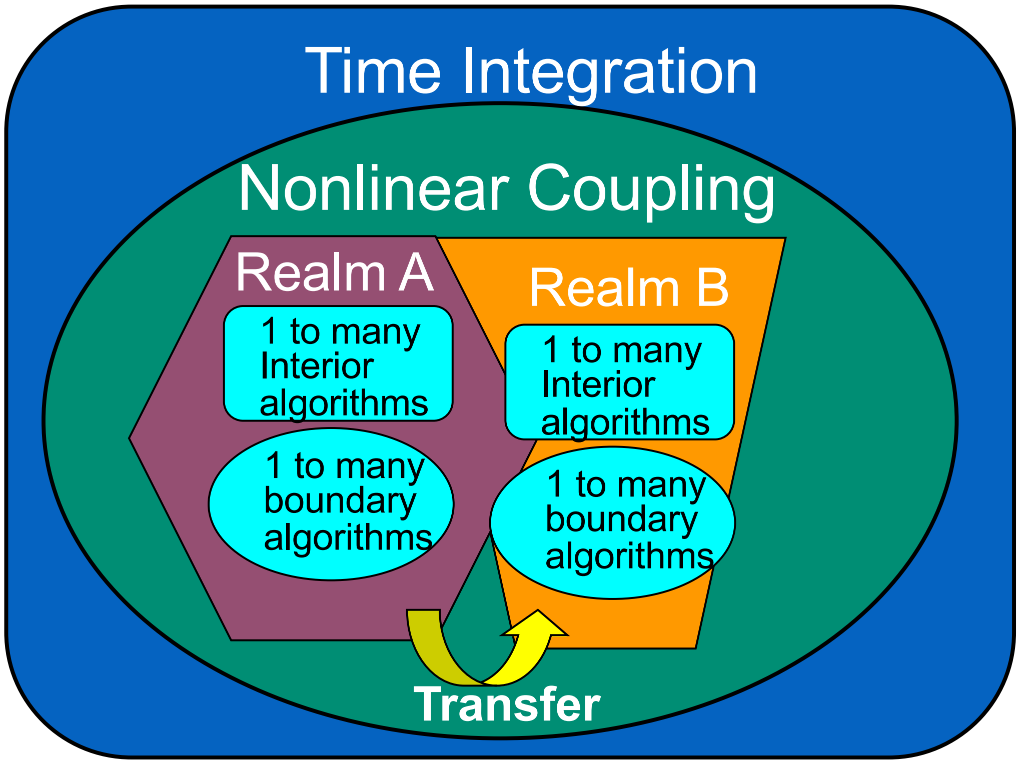





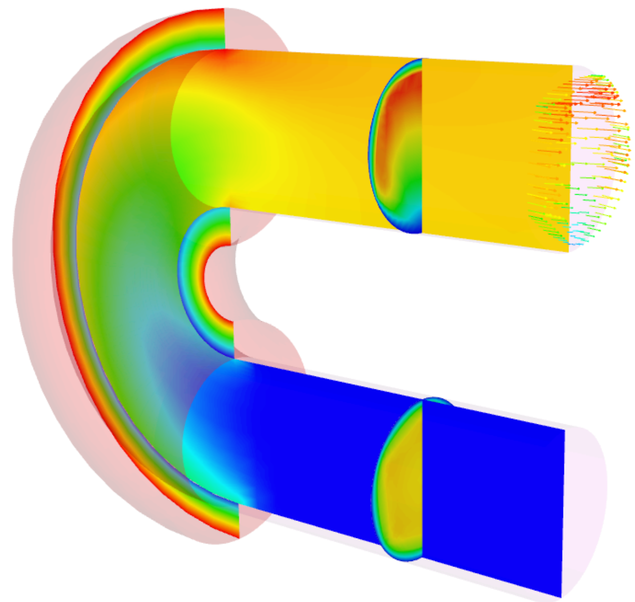

Vertical Axis Wind Turbine (VAWT)

Horizontal Axis Wind Turbine (HAWT)

# 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: Specification of sparse Trilinos-based precond/solver

transfers: Data transfer for multi-physics coupling

realms:

*YAML enforces strict spacing and ordering*

https://www.democraticunderground.com/10021540110

```
  - 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
```

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
```

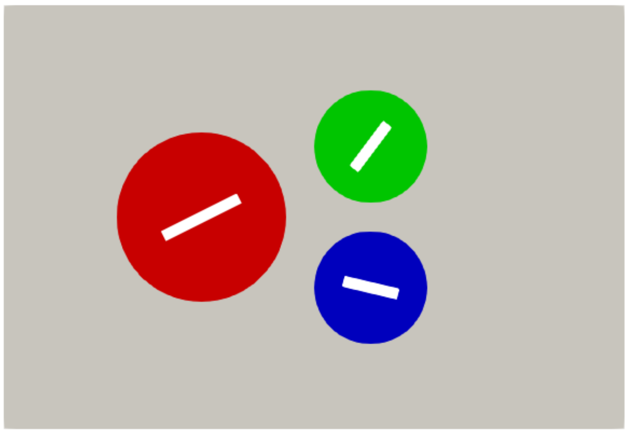
```
material_properties:

  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
```

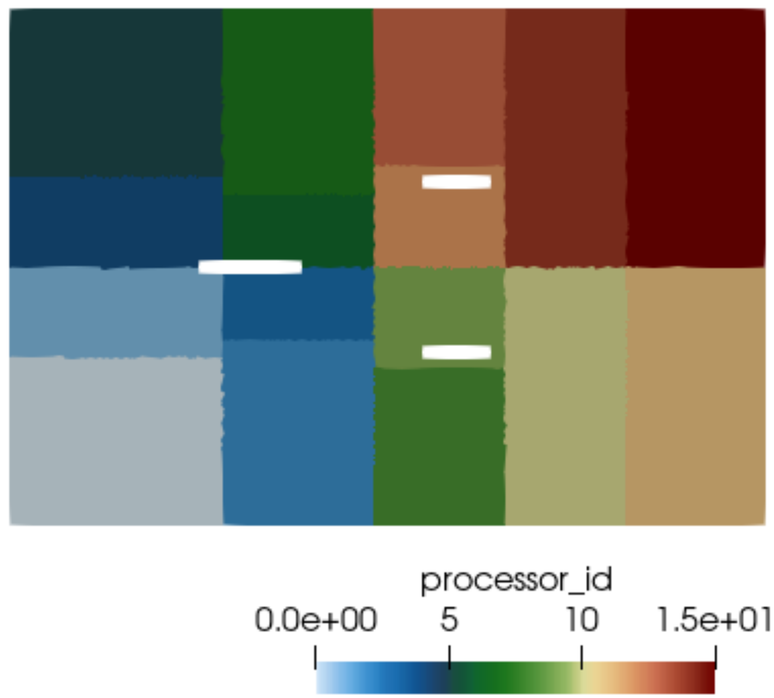
# A Note on Parallel Decomposition

- As noted, decomposing the mesh into small subsets and operating on these subsets in parallel provides a methodology for increased simulation time



Colored by block ID

Colored by core count (= 1) One mpi rank.




16 MPI ranks = 16x faster (hopefully)

# How to Run in Parallel: Mesh Decomposition

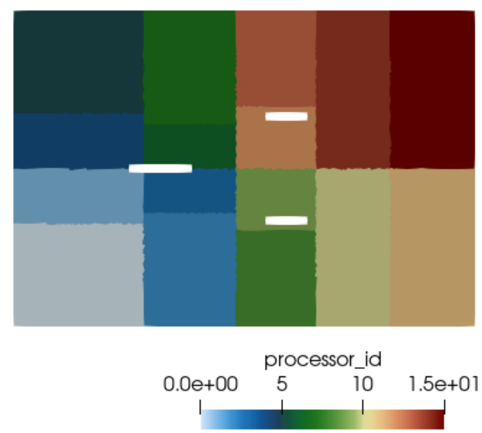
- Given a mesh, mesh.g and myInputFile.i, if one desires to run on, e.g., 16 core case:

1. Use pre-processing "decomposition" tools (Trilinos/install/bin)
2. In-situ

myMesh.g

>/path/to/decomp -j {np} {meshName}
>mesh.g.16.00, mesh.g.16.01, .., mesh.g.16.15

1: - name: realmFluids
mesh: mesh/myMesh.g
~~automatic_decomposition_type: rcb~~




2: - name: realmFluids
mesh: mesh/myMesh.g
automatic_decomposition_type: rcb

>mpirun --np 16 /naluPath/naluX -i input.i &

>results.e.16.00, results.e.16.01, .., results.e.16.15
>input.log

# A Note on Divergence

- Whether by design or poor code usage, solution results from CFD analysis for complex applications may diverge. How do I know?

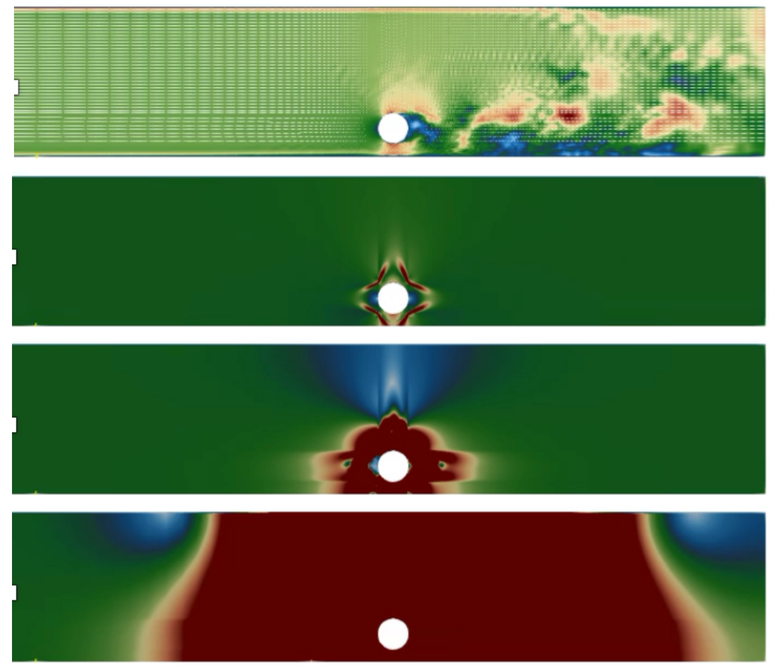
1. Non-finite residuals, i.e., not-a-number:“nan” (either linear or non-linear),

```
const double norm = 0.0;
const double flux = rho*u*A/norm;
```

2. Simulation runs, however, results look very wrong

- Typical causes?

1. Bad initial condition that drives nonlinear solution to diverge
2. Too large of an initial time step
3. Poor stabilization, numerical parameters, etc.
4. Poor time integration
5. Ph.D. from ICME explaining why…



EBVC flow-past 2D cylinder
Top: +NOC
Bottom se: -NOC

# 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:

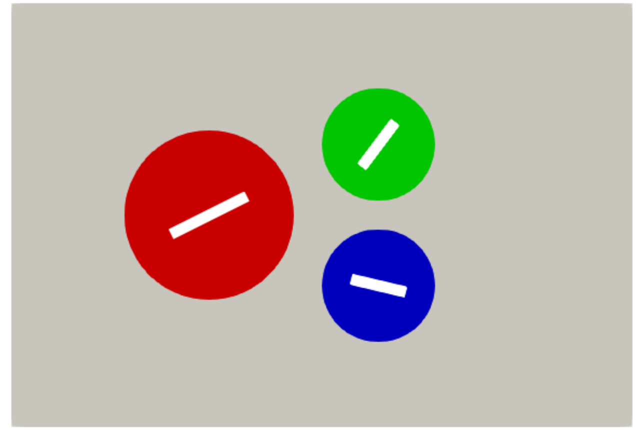
1. Nalu/reg_tests/test_files/dgNonConformalThreeBlade
2. Nalu/reg_tests/test_files/fluidsPmrChtPeriodic
3. Homework #1:
   1. https://github.com/spdomin/Present/tree/master/standformMe469/hwOne

- 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

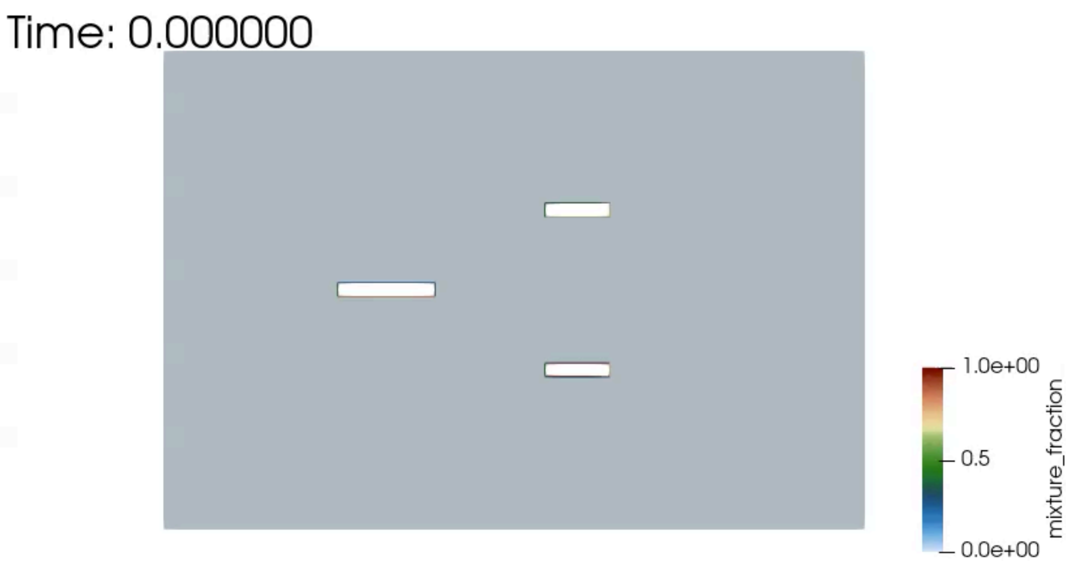
Resource: https://nalu.readthedocs.io/en/latest/source/theory/index.html

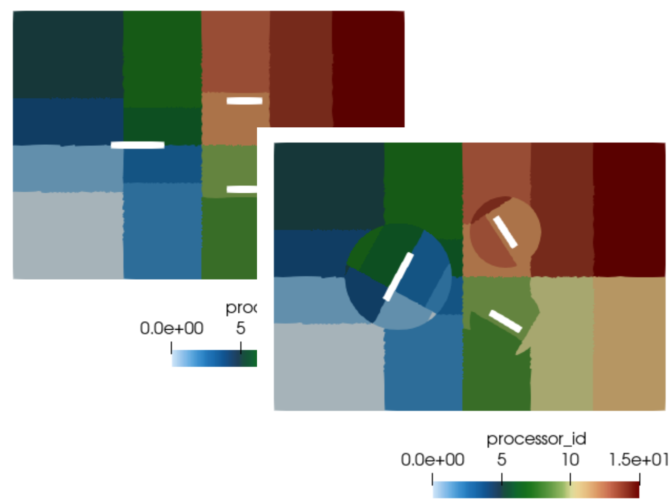
# Nalu/reg_tests/test_files/dgNonConformalThreeBlade

- 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

$U\Delta t / \Delta x$

$\gamma_i$ 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
```

$\rho U L / \mu$

```
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
```

equations

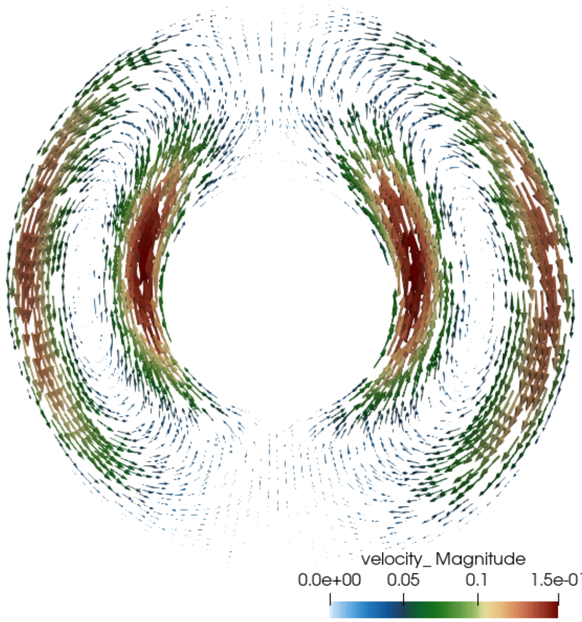
nonlinear iterations

```
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
```

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

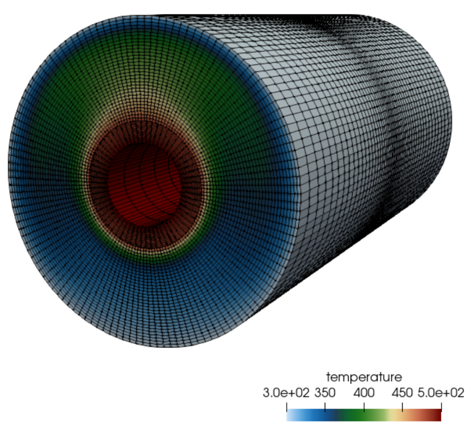


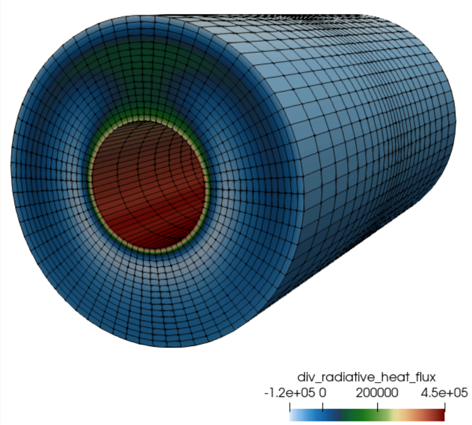

Stark#, cond/rad

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

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

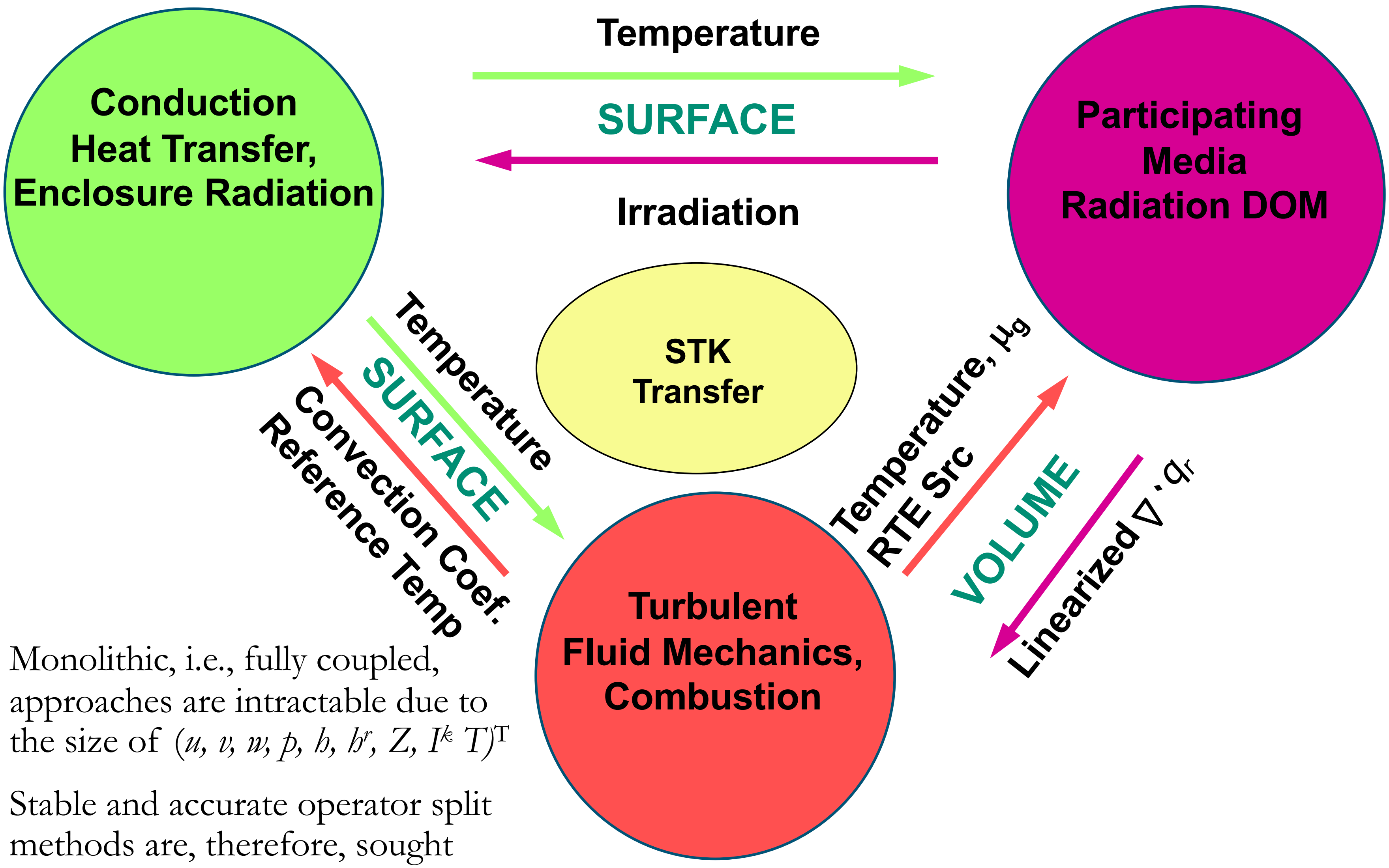
$Ra = g\ \beta\ (T_i - T_o)\ L\ /\ Pr\ \alpha^2 \sim 2e6$




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

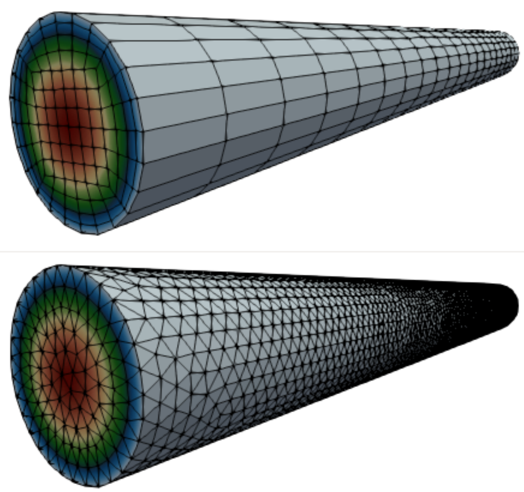
# Nalu/reg_tests/test_files/fluidsPmrChtPeriodic




- 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

# Laminar Pipe Flow: Specified Pressure Drop for $Re^{\tau}$= 10

- 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
  - $\rho$ = TBD
  - $\mu$ = TBD
  - dp/dz = TBD
  - Uc = TBD



# Break-out Example Using Paraview

- Live in-class demo

# 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
- Multi-physics by design (operator split)
- Funded through ASC, ECP, A2e, ASCR, and LDRD
- Elements of an input file
  - Solvers, mesh, equations, material models, boundary conditions, etc.
- The need for parallel computing
- Examples
  - Fixed rotation for three blades
  - Thermal/PMR/Fluids
- Paraview to visualize