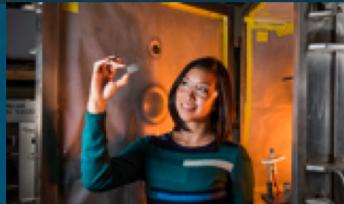
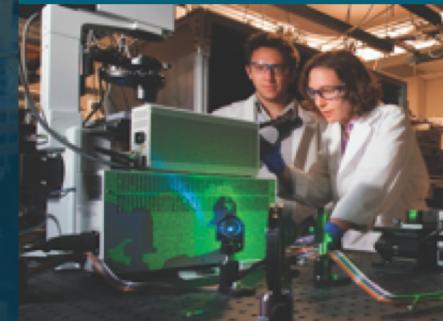


Guest Lecture Stanford ME469: Nalu Overview



Sandia
National
Laboratories



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

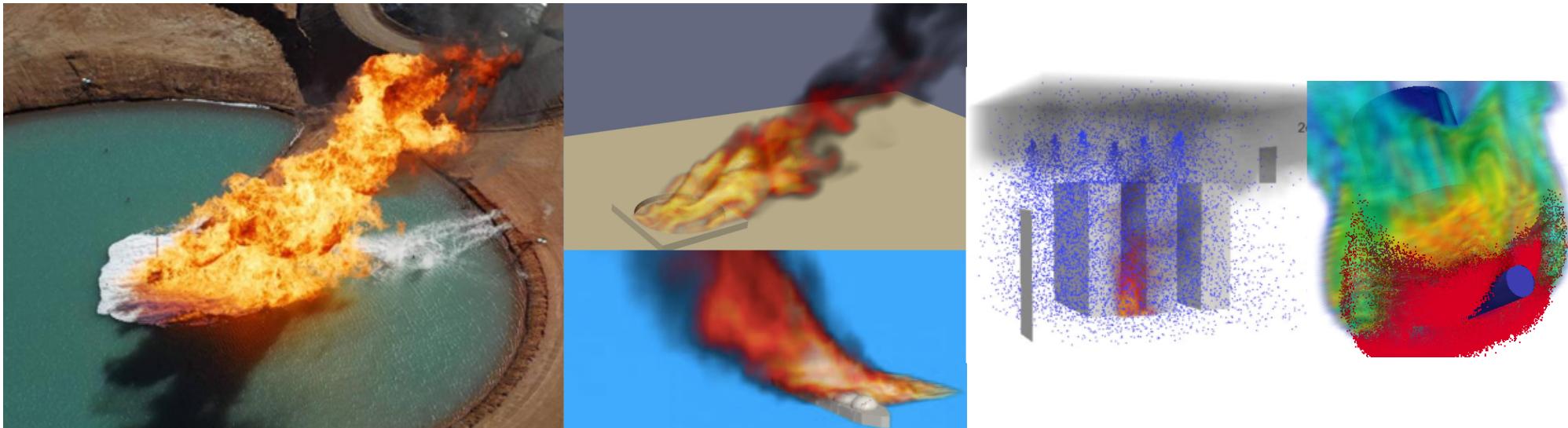


- Nalu Technology Origination: ASC
- Beyond the 32-bit Limit
- Supported Physics
- Supported Numerics
- Low- and High-order
- Moving Mesh (Sliding and Overset)
- Multiphysics:
 - Fluid Structure Interaction
 - Conjugate Heat Transfer (CHT)
 - Participating Media Radiation
- Examples
- Conclusion

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

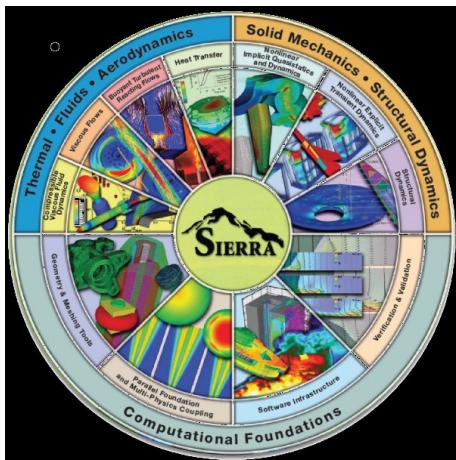


- Complex geometry has driven a generalized, hybrid unstructured discretization approach supporting Hex8, Tet4, Wedge6, and Pyramid5 elements in addition to arbitrary promotion of Hex8 to Hex27, Hex64, etc.

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 are not yet known

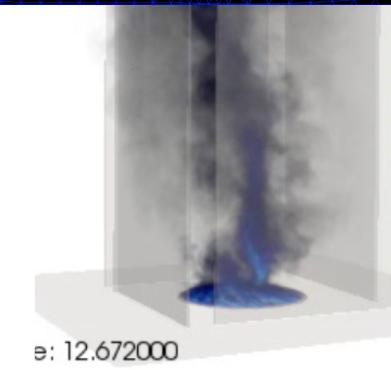
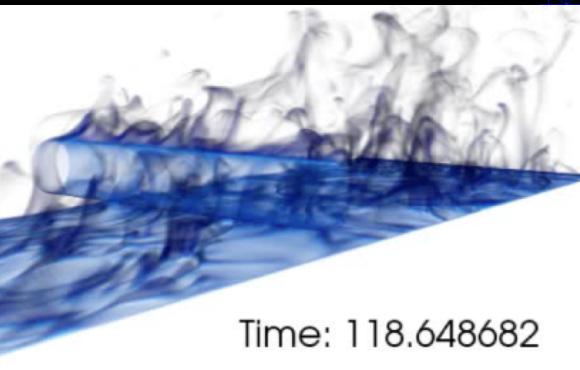
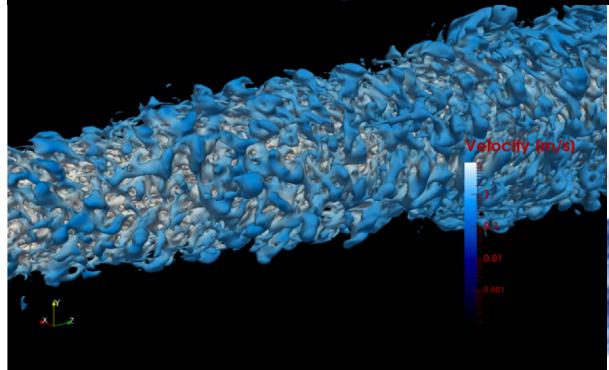
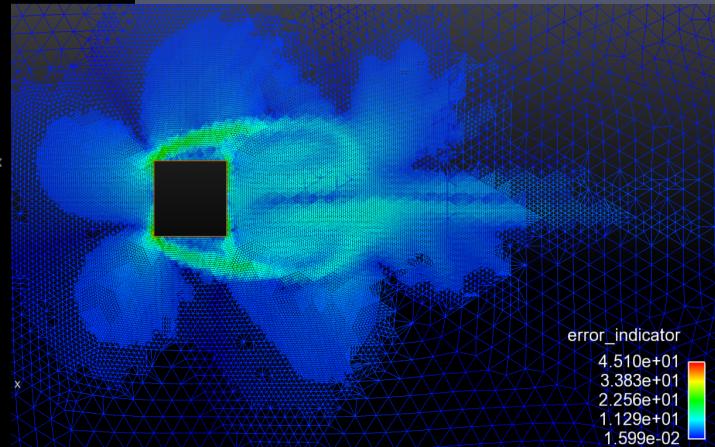
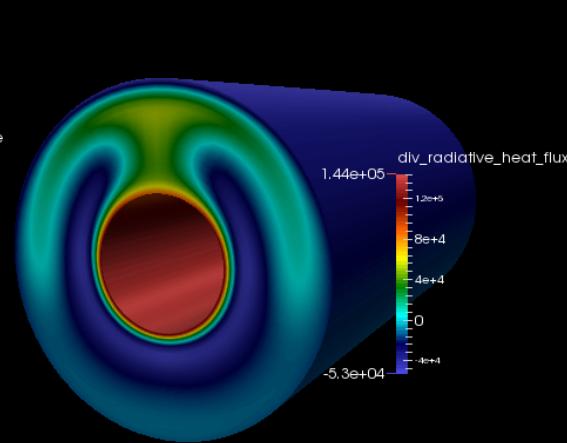
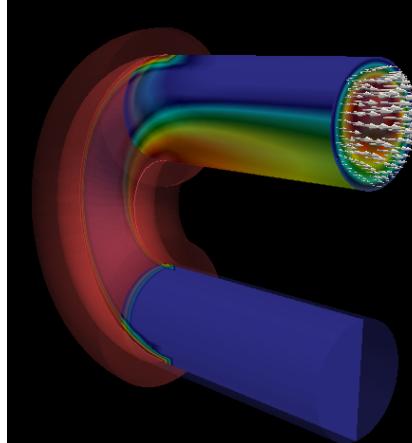
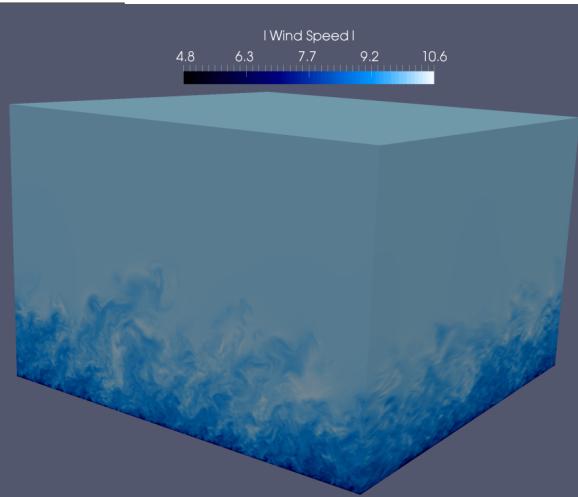
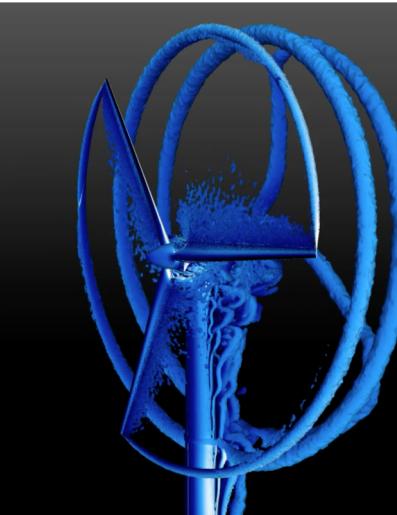


+ ASC IC
Investments



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

Supported Physics



6 Developed Open-Source BSD-clause 3 Distribution Policy



- Philosophy: Open-source collaborations



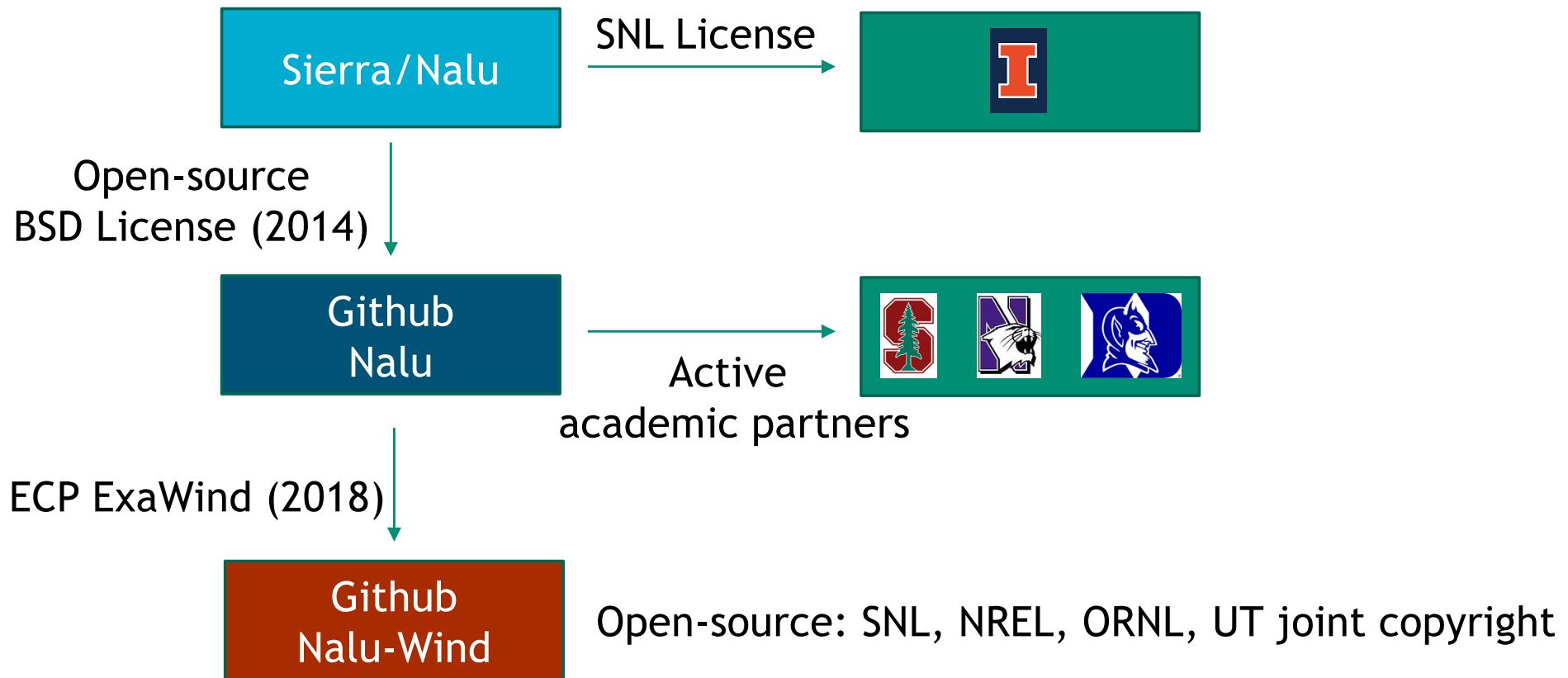
<https://github.com/NaluCFD>



Nalu History



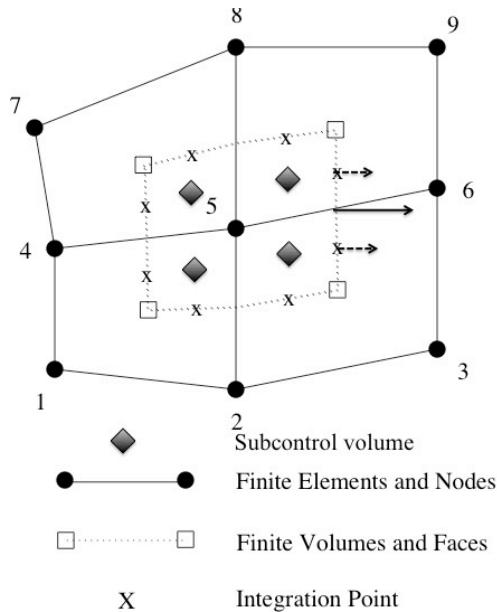
- A time-history of the Nalu code base:
- By CFD standards, this is a relatively new code base



Supported Discretizations: CVFEM/FEM/EBVC



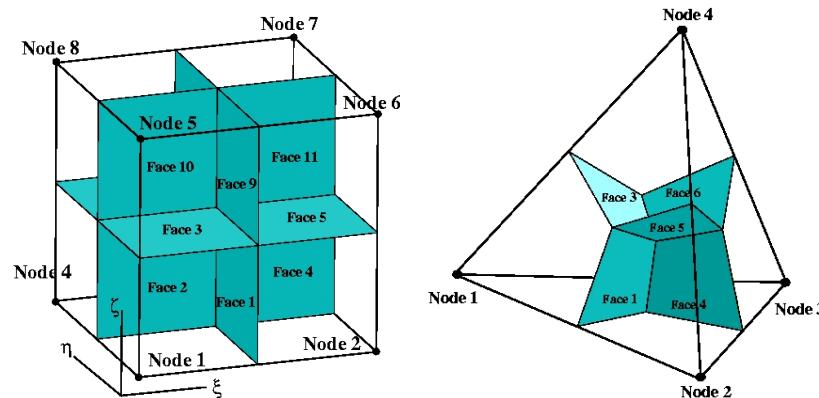
- The core discretization used in the low Mach code base has been the Control Volume Finite Element Method, CVFEM
- Finite Element Method and Edge-based Vertex-Centered, EBVC, are also supported



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

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

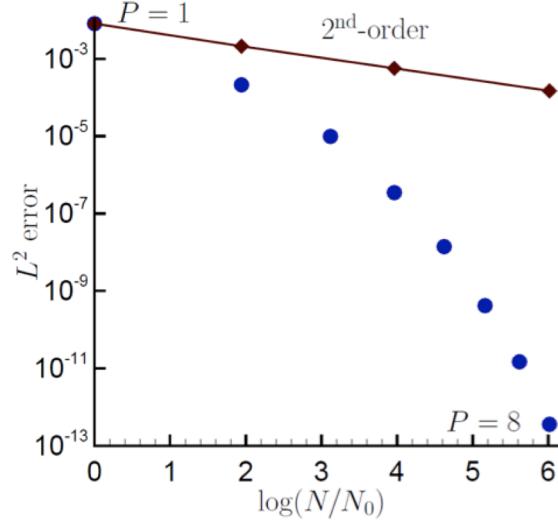
$$\int w \frac{\partial \bar{\rho} \tilde{u}_j \tilde{\phi}}{\partial x_j} d\Omega = \sum_{ip} (\bar{\rho} \tilde{u}_j)_{ip} \tilde{\phi}_{ip} n_j dS = \sum_{ip} \dot{m}_{ip} \tilde{\phi}_{ip}$$



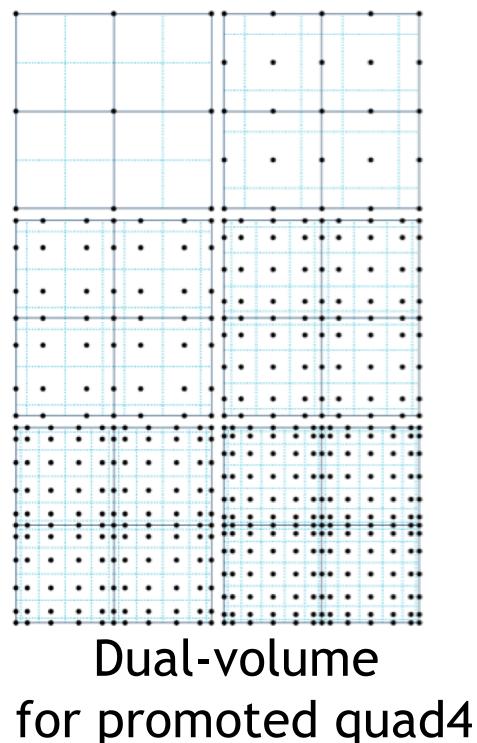
Scientific Research Platform to Evaluate Higher-Order Methods on Next Generation Platforms

9

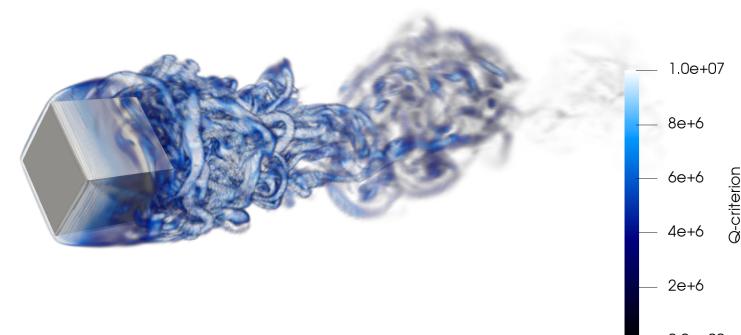
- As the cost of parallel assembly increases, should we strive to perform more local work? Higher-order achieves this design-point (at the cost of a larger memory footprint)



Spectral convergence



Time: 0.055000



Time: 0.055000

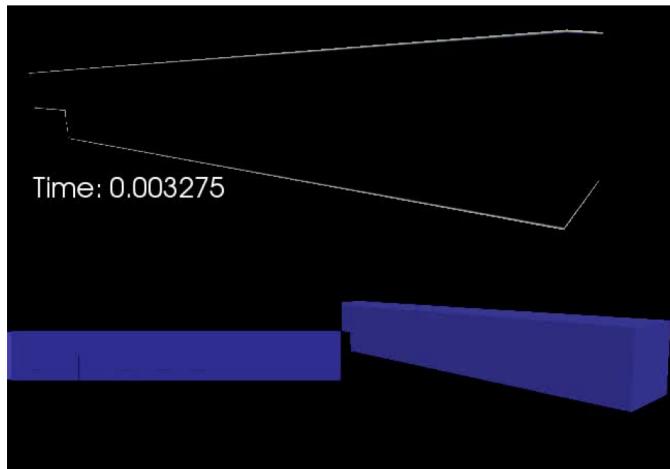


Flow-past rotating cube
Re~4000, RPM~3200
Same node count,
 $P=1$ (top) $P=2$ (bot)

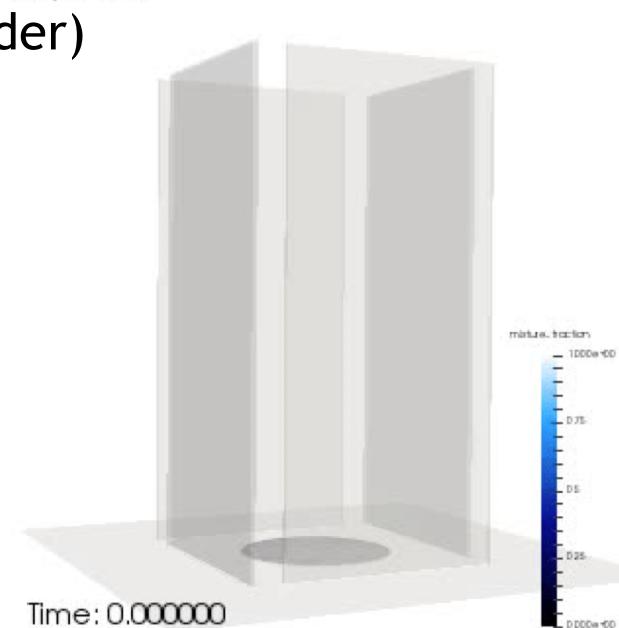
Several Multi-physics Flow Examples



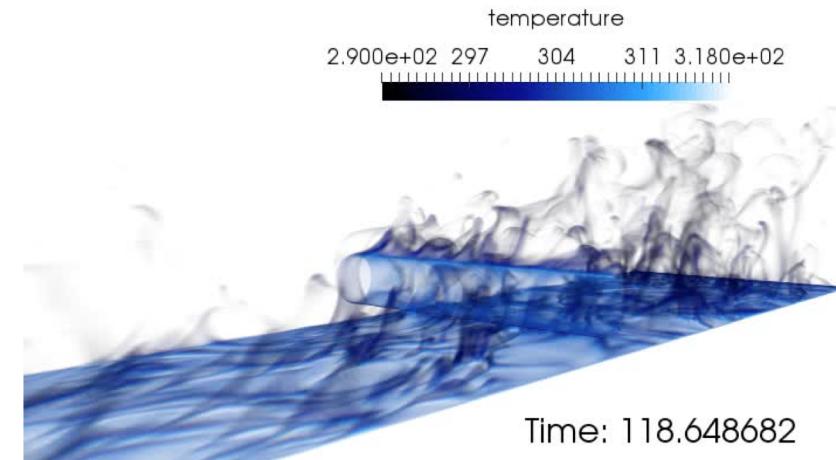
Helium plume (low-/high-order)
R1, 20cm



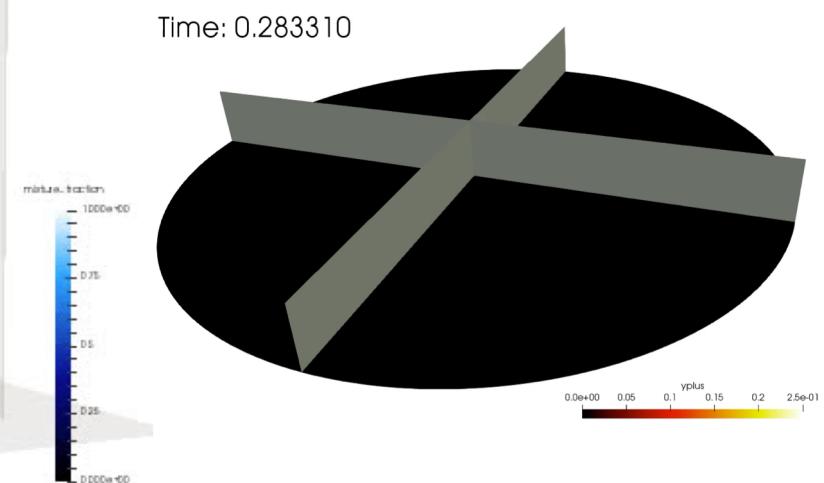
Heated backstep



Whirling behavior



Cylinder in cross flow



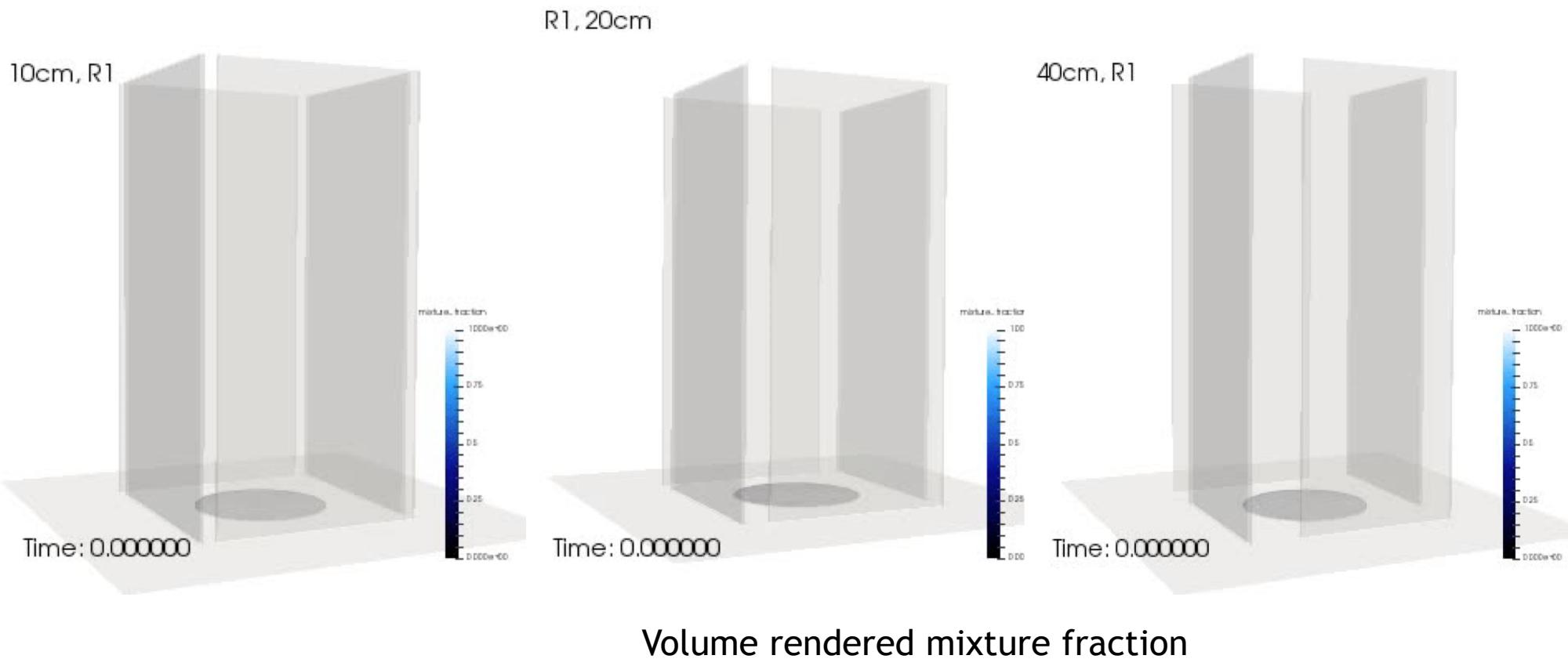
Impinging Jet DNS

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

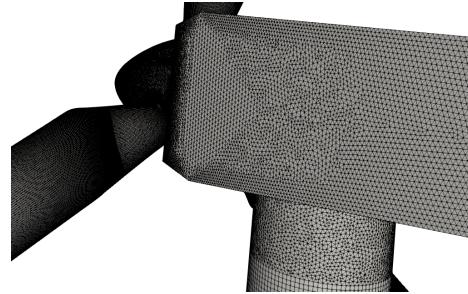


SAND2019-7052 C

- 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?

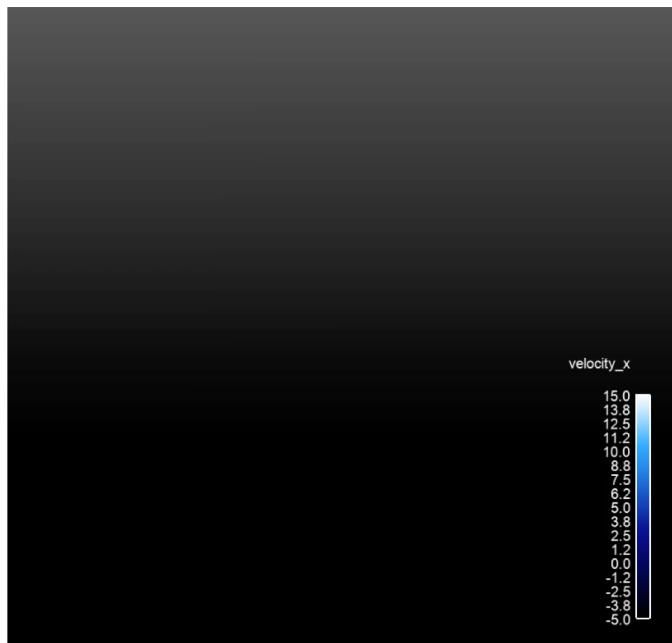
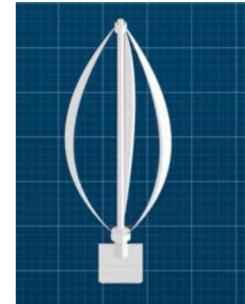


Unique Wind Energy Needs

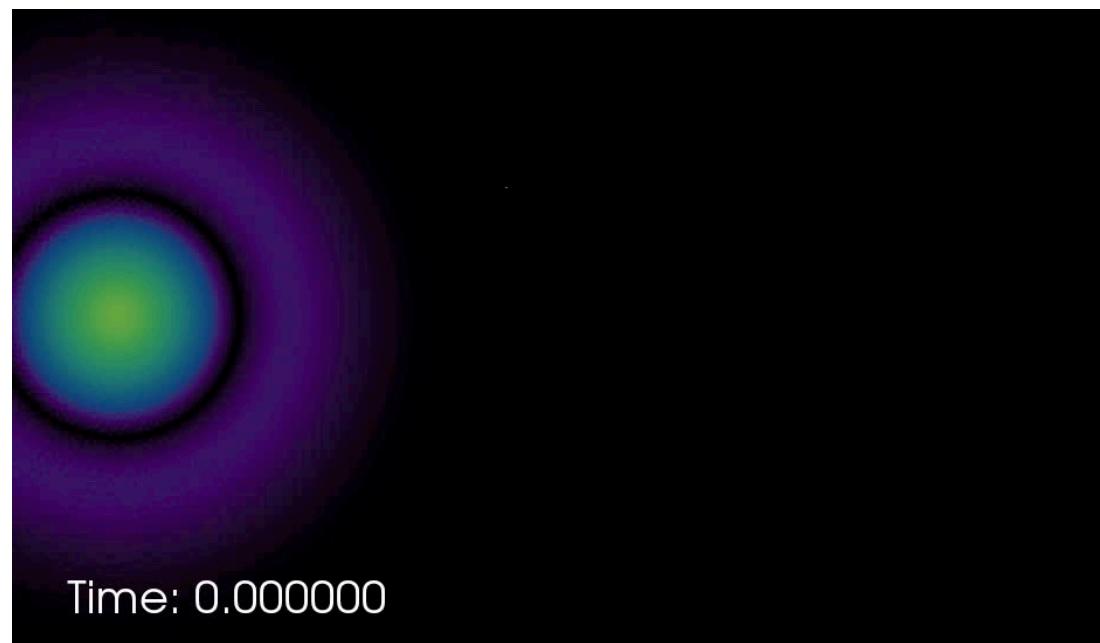


- Low-dissipation methods with suitable nonlinear stabilization operators to perform blade-resolved physics
- Complex rotating blades, pitching blades, with possible yaw
- Transition from low-order (near the blade) to higher-order (in the wake)

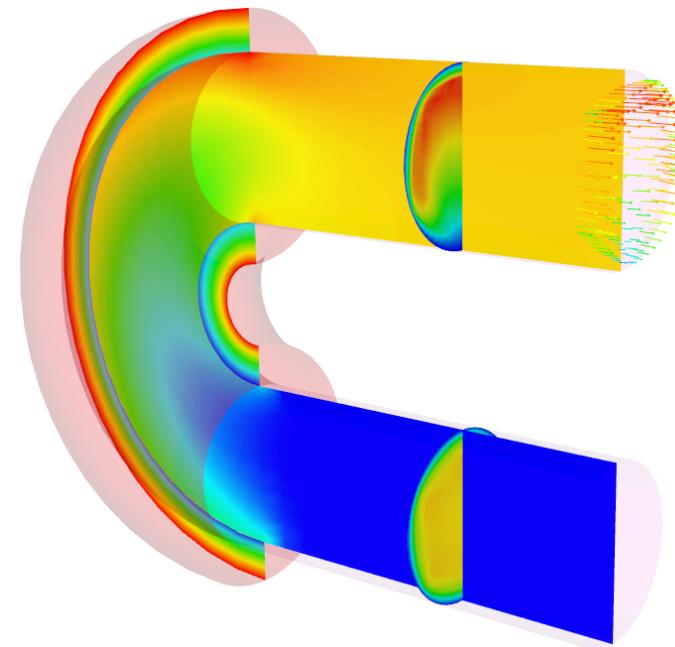
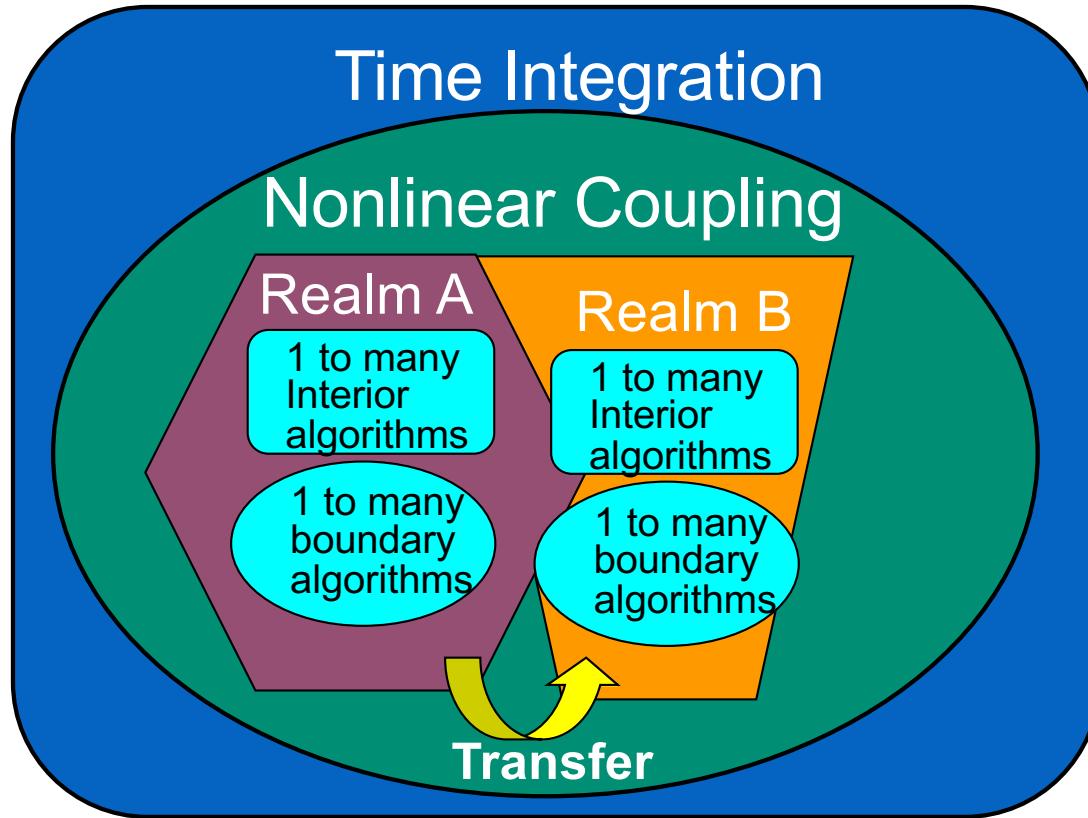
Generalized, unstructured, hybrid low-order simulations shown



Horizontal Axis Wind Turbine
(HAWT)



Vertical Axis Wind Turbine
(VAWT)



- *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

- 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: ← Time integration, e.g., BE, BDF2



<https://www.democraticunderground.com/10021540110>

Physics definitions

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



- 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:

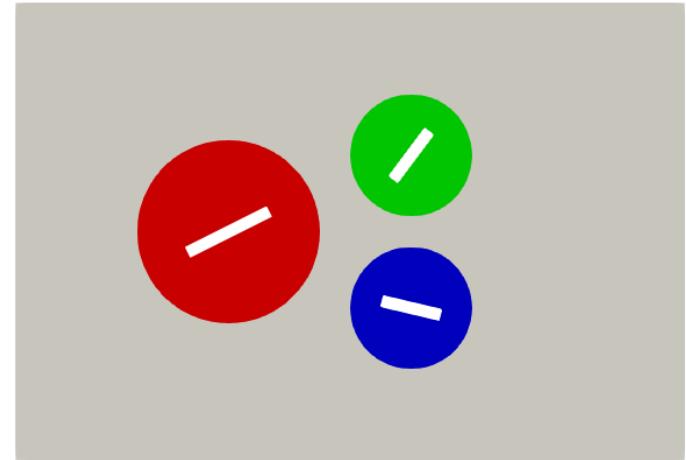
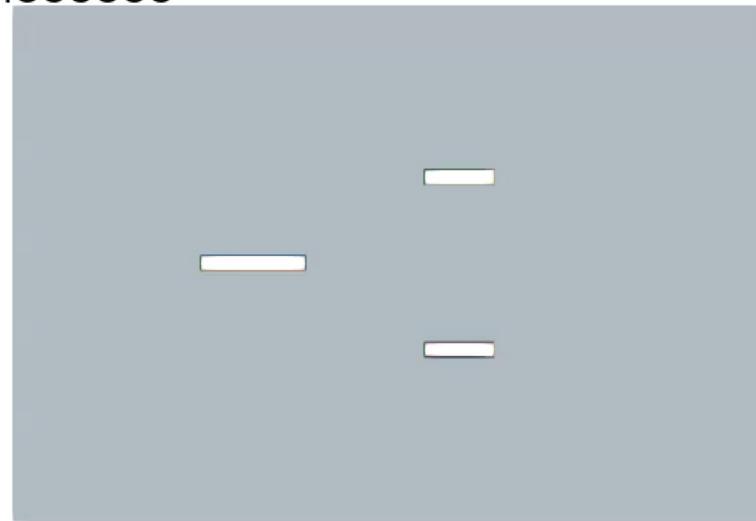
1. Nalu/reg_tests/test_files/dgNonConformalThreeBlade
2. Nalu/reg_tests/test_files/fluidsPmrChtPeriodic
3. Homework #1:
 1. <https://github.com/spdomin/Present/tree/master/standformMe469/hwOne>
 - Feel free to run any case that you feel looks interesting to you!
 - Note that the regression test suite 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

Time: 0.000000



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

$\rho U L / \mu$

realm_1::advance_time_step()		Linear Iter	Linear Res	NLinear Res	Scaled NLR
---	---	-----	-----	-----	-----
1/2	Equation System Iteration				
1/1	myLowMach	4	1.27653e-07	0.000173716	1
	MomentumEQS	9	5.17721e-06	0.00618278	1
	ContinuityEQS	19	4.2818e-09	2.78318e-06	1
	PNGradPEQS	20	9.70201e-09	5.20951e-06	1
	PNGradUEQS				
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

nonlinear
iterations

equations

Mass Balance Review:

Density accumulation: 0

Integrated inflow: -0.375

Integrated open: 0.3749998354138842

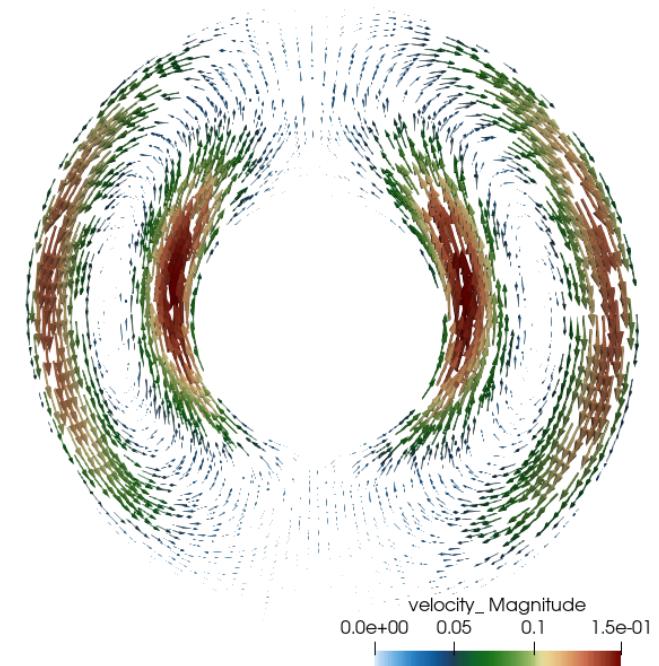
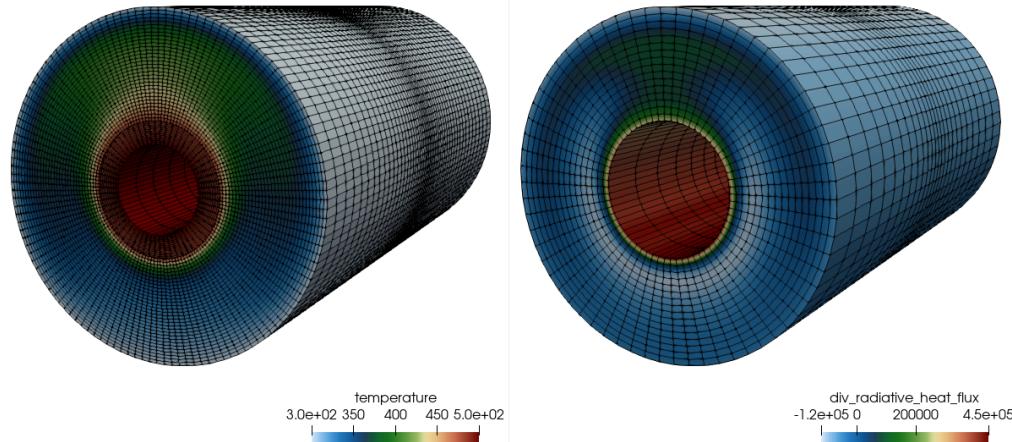
Total mass closure: -1.64586e-07

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



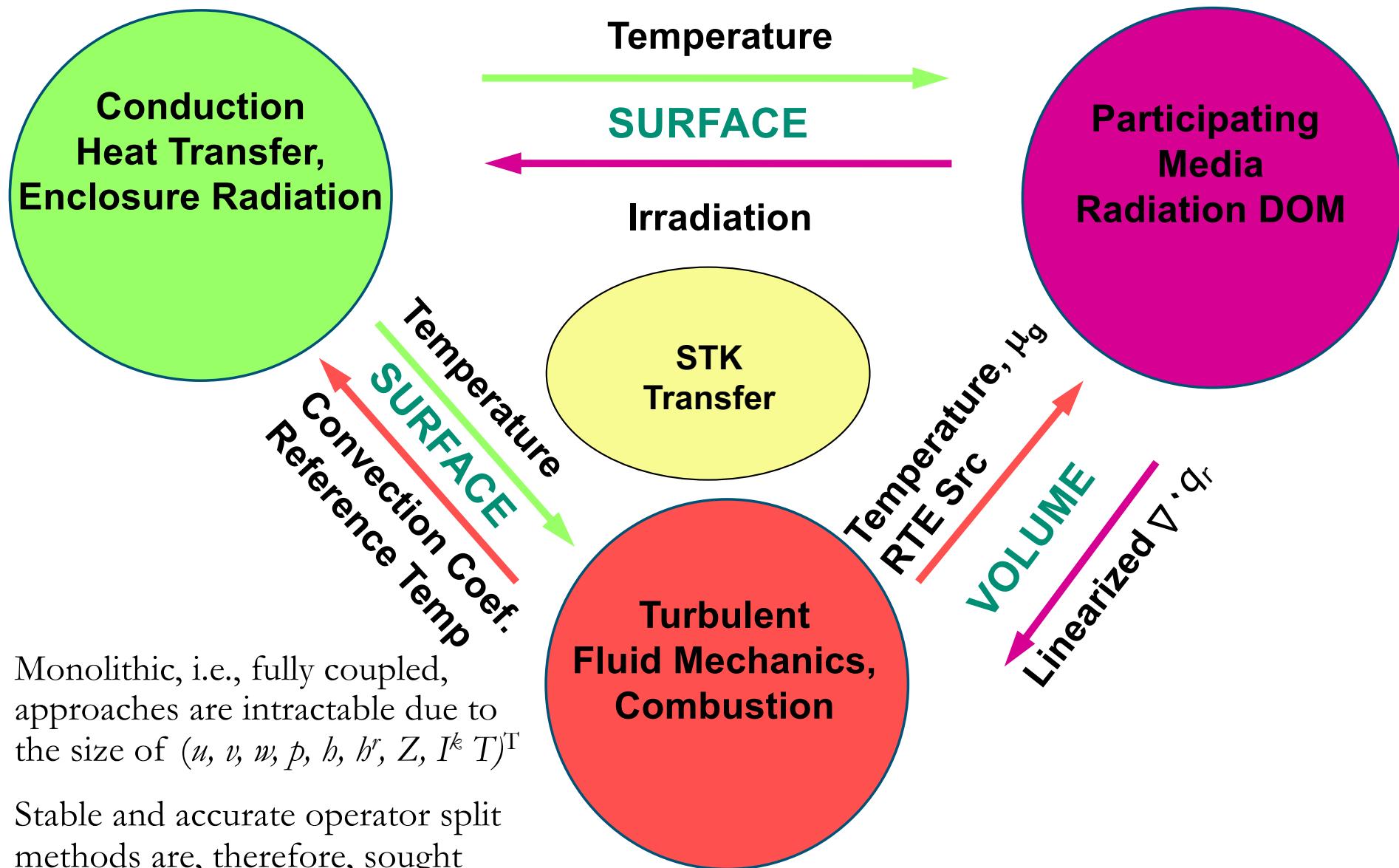
$$\text{Stark\#}, \text{cond/rad}$$

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

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

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

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



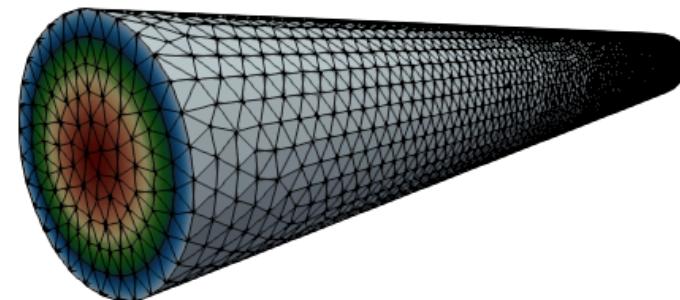
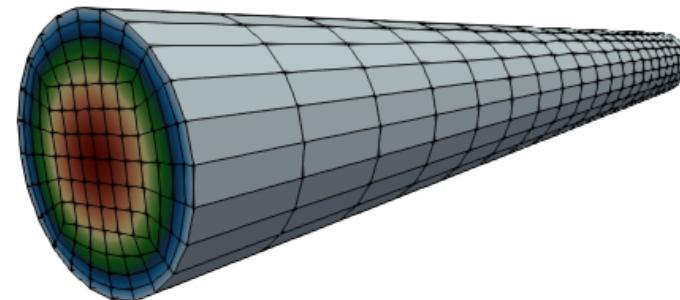
- Monolithic, i.e., fully coupled, approaches are intractable due to the size of $(u, v, w, p, b, b^r, Z, I^k T)^T$
- Stable and accurate operator split methods are, therefore, sought
 - See Domino et al., *AIAA*, 2007



- 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/standformMe469/hw/one>

- Specifications:
 - $Re^{\tau} = 10$
 - Pipe diameter, $D = 0.01 \text{ m}$
 - Pipe Length, $L = 0.2 \text{ m}$
 - $\rho = \text{TBD}$
 - $\mu = \text{TBD}$
 - $dp/dz = \text{TBD}$
 - $U_c = \text{TBD}$





- 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