INL/CON-24-78631-Revision-0

Development of Segregated Thermal-Hydraulics Solvers in MOOSE

June 2024

Changing the World's Energy Future

Peter German, Mauricio Eduardo Tano Retamales, Alexander D Lindsay, Ramiro Oscar Freile, Guillaume Louis Giudicelli, Sebastian Schunert

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Development of Segregated Thermal-Hydraulics Solvers in MOOSE

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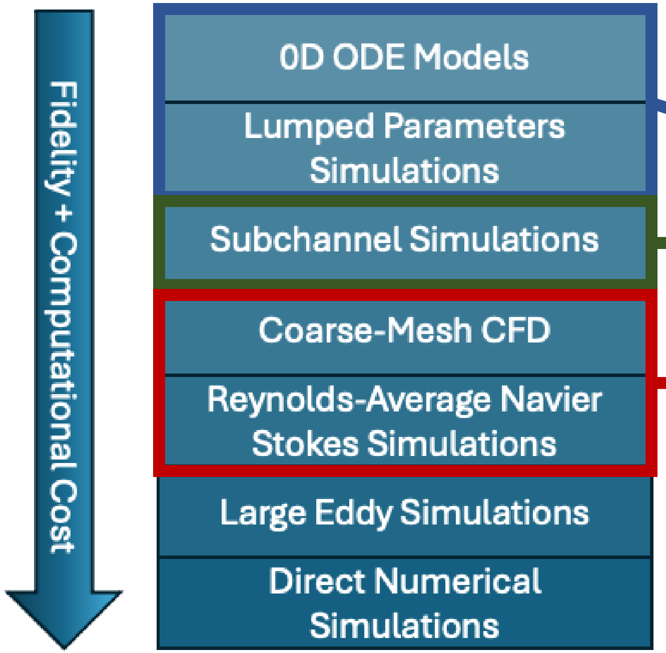
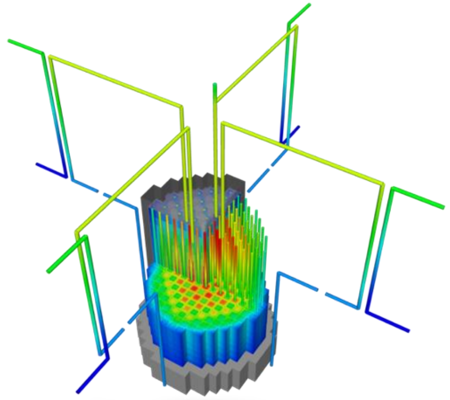
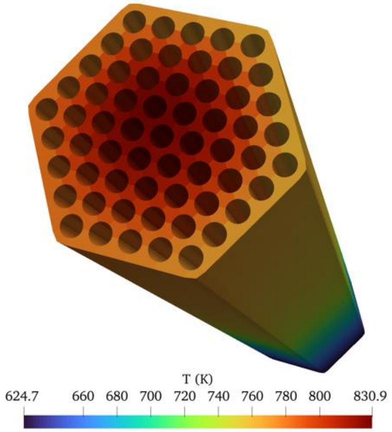
Thermal-hydraulics in MOOSE

- Multiphysics Object-Oriented Simulation Environment (MOOSE) provides a set of opensource tools (modules) for thermal-hydraulics simulations at different length scales
- Supported by Nuclear Energy Advanced Modeling and Simulation (NEAMS) program
- Other NEAMS thermal-hydraulics applications harnessing MOOSE: SAM, Cardinal, Pronghorn

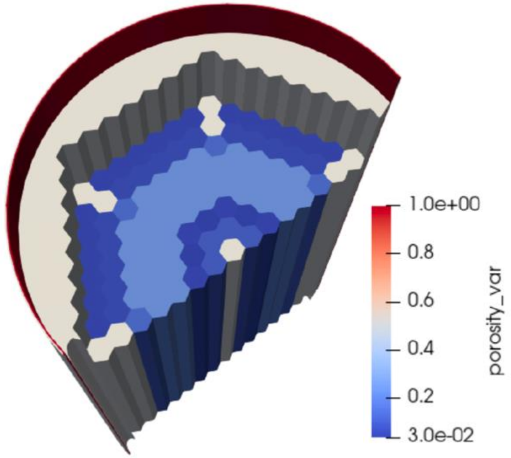


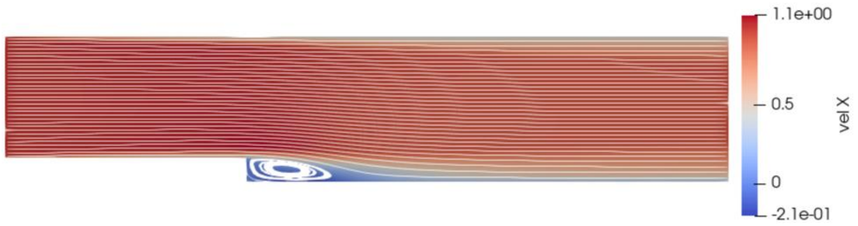


Thermal-Hydraulics Module (THM)



Subchannel Module (coming soon)





Navier-Stokes Module

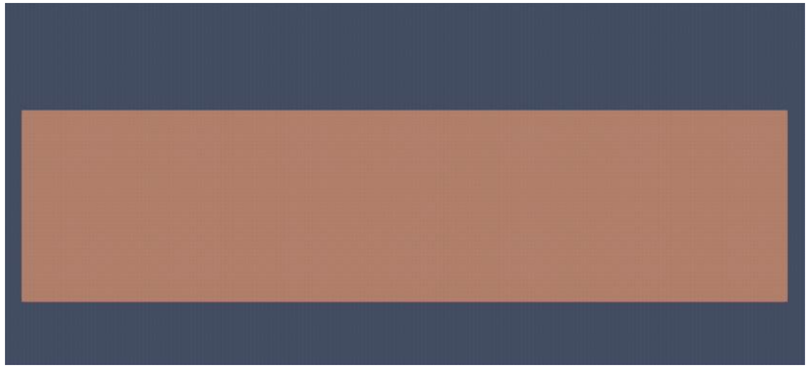
MOOSE – Navier-Stokes Module

- Supported spatial discretization:
  - Stabilized Finite Element Method: 2017 –
  - Finite Volume Method: 2021 –
  - Hybridized Discontinuous Galerkin Finite Element Method: 2024 –

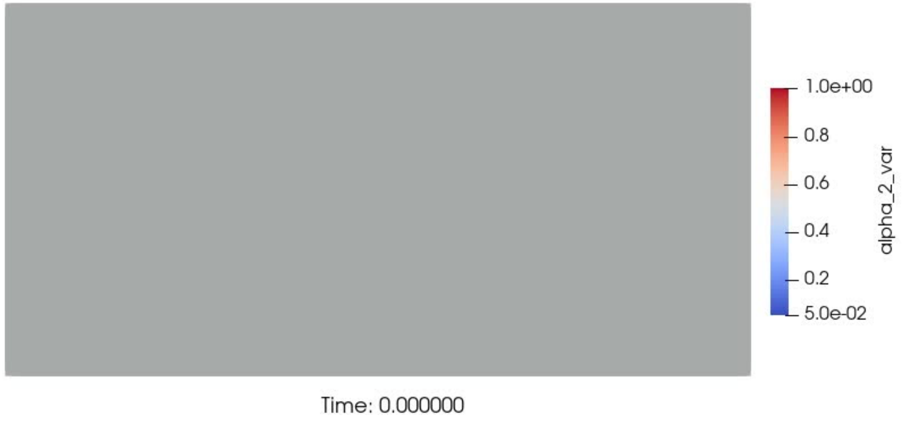
- Fluid types:
  - Incompressible
  - Weakly-compressible
  - Compressible

- Flow regimes
  - Laminar
  - Turbulent (RANS)

- Flow types:
  - Free-flow
  - Porous medium flow
  - Two-phase flow



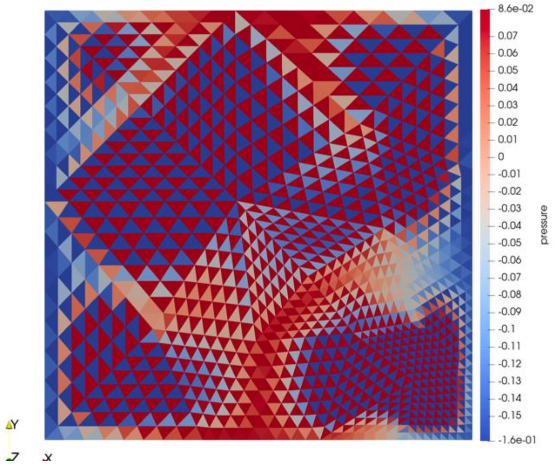
Simulation of laser melt pool using Arbitrary Lagrangian-Eulerian formulation (ALE)



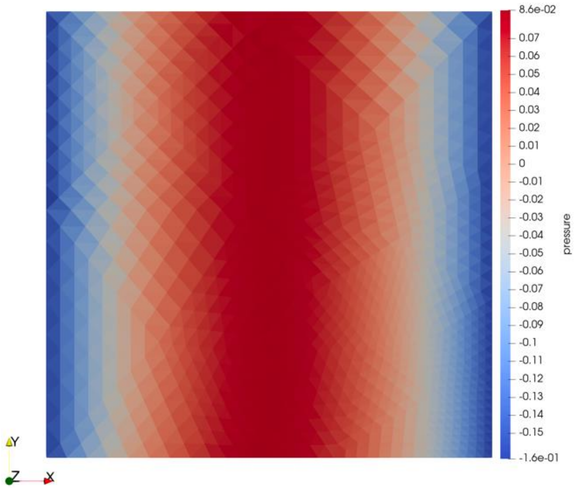
Phase separation from mixture in a channel

Motivation – Challenges

- Newton's method using tightly coupled problems can become computationally expensive (both in CPU and memory usage), especially for 3D problems
- Due to the saddle point problem in the incompressible formulation, a full LU preconditioning was used on the Jacobian (scales poorly with number of cells)
- Unclear if Schur-complement-based field split preconditioners are sufficient due to the Rhie-Chow interpolation (needed to avoid pressure checkerboarding)



$$u_{RC} = u_{AVG} - \left(\frac{1}{a}\right)_f (\nabla p_f - \overline{\nabla p})$$



SIMPLE, a segregated solution algorithm, was added to the Navier-Stokes module:

- The individual systems are easier to precondition
- The Picard-style solution algorithms allow much sparser systems by lagging gradient-related terms
- Allows flexible equation relaxation for more robust solves

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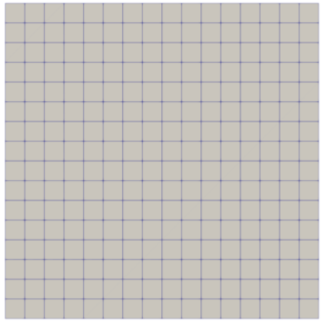
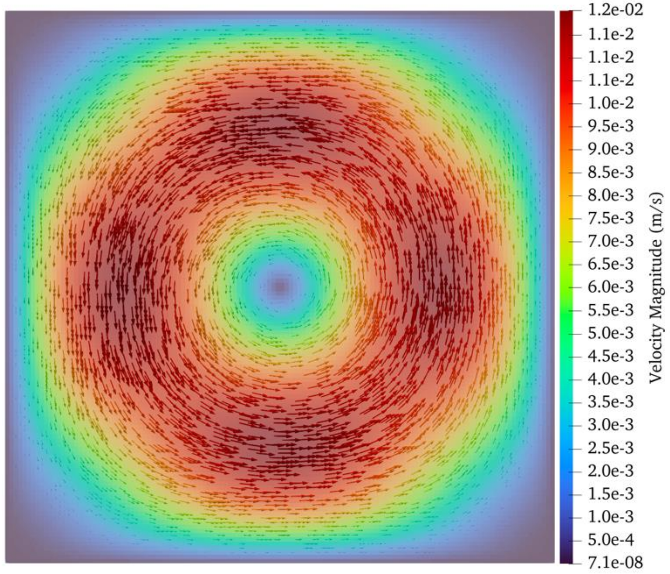
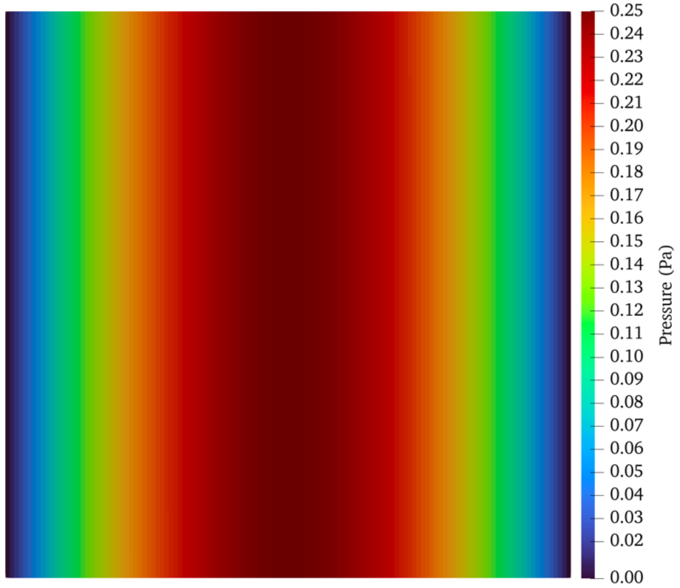
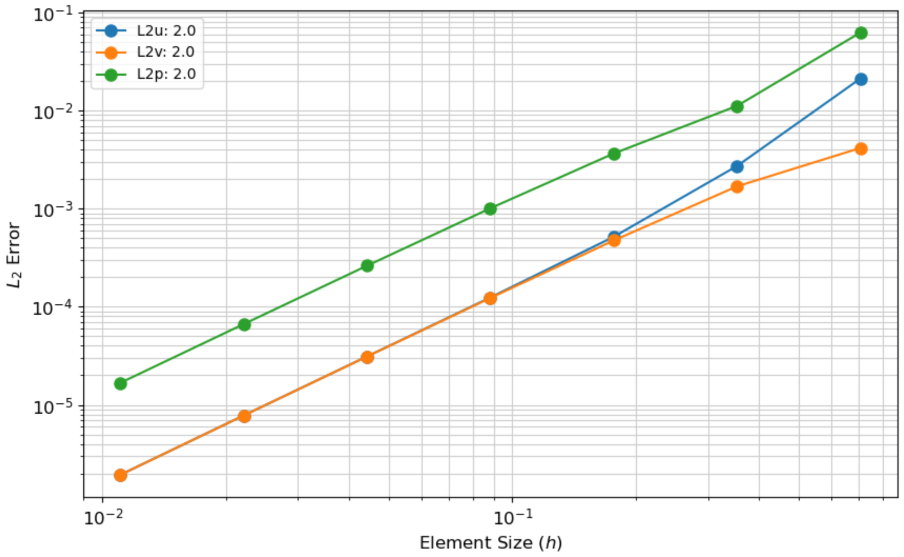
Verification using Method of Manufactured Solutions

- 2D laminar vortex problem
  - Orthogonal grid, weighted average advection scheme, Dirichlet BCs
  - Expected convergence rate: $O(h^2)$ in velocity and pressure



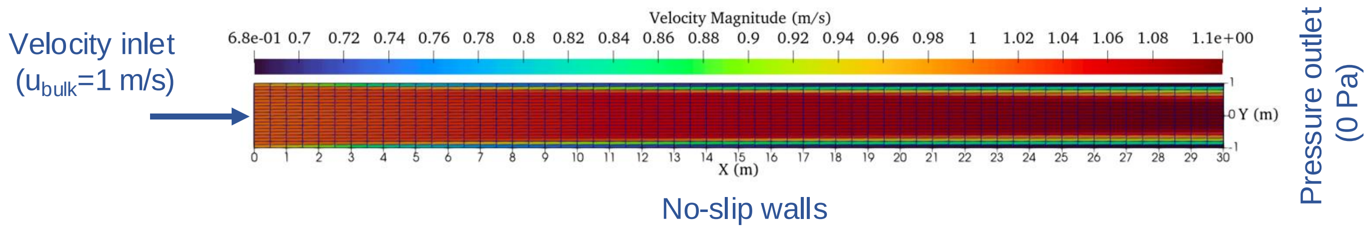


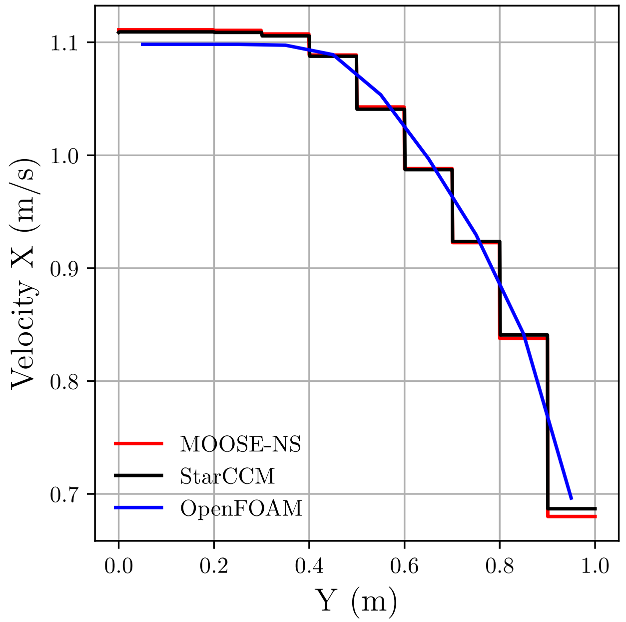




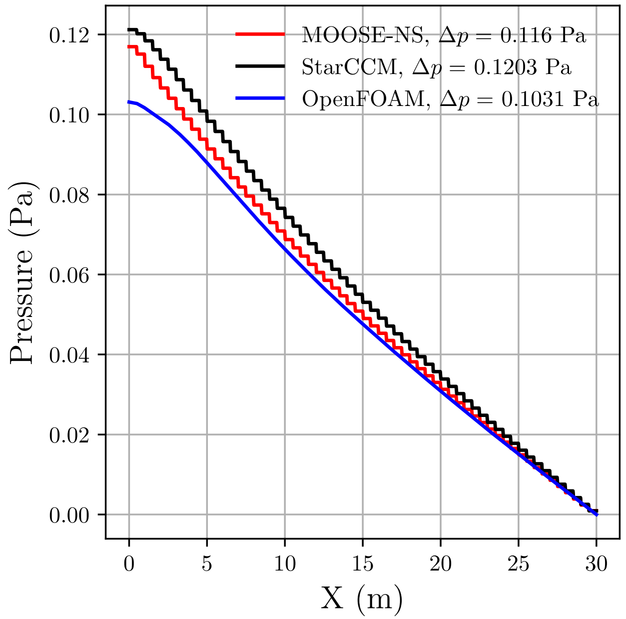
Code-to-code comparison – channel flow

- 2D Turbulent flow:
  - Re=18,000
  - Standard k-epsilon model
- Tested with:
  - Star-CCM+
  - OpenFOAM
  - MOOSE Navier-Stokes module
- Same mesh, same discretization settings
- Comparing:
  - Velocity profiles at the outlet
  - Axial pressure drop at the middle plane





Velocity profile at outlet



Axial pressure drop at the middle plane

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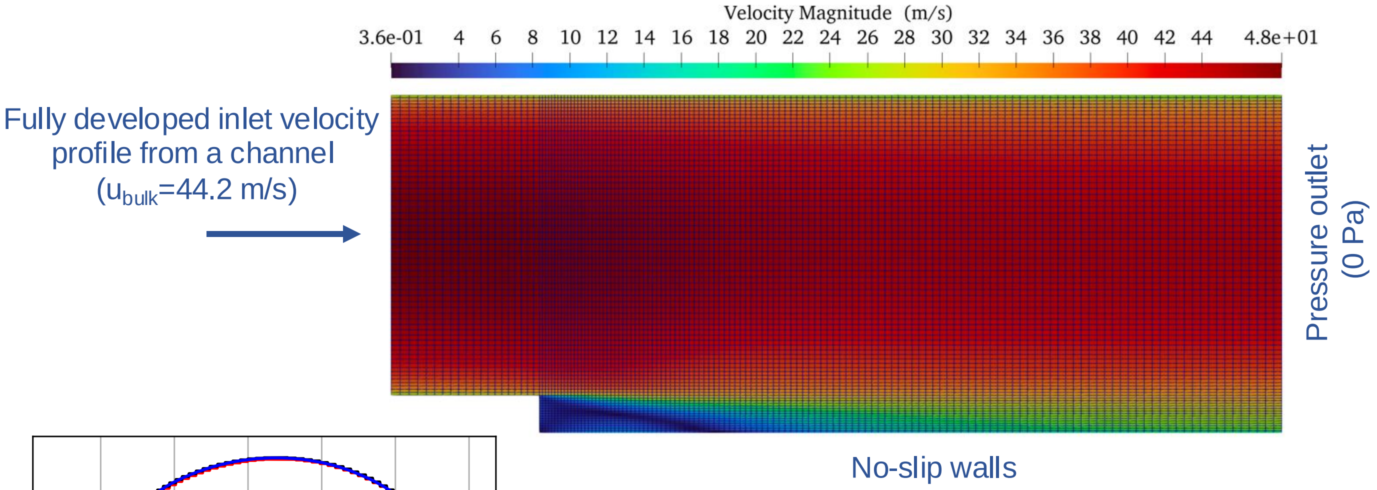
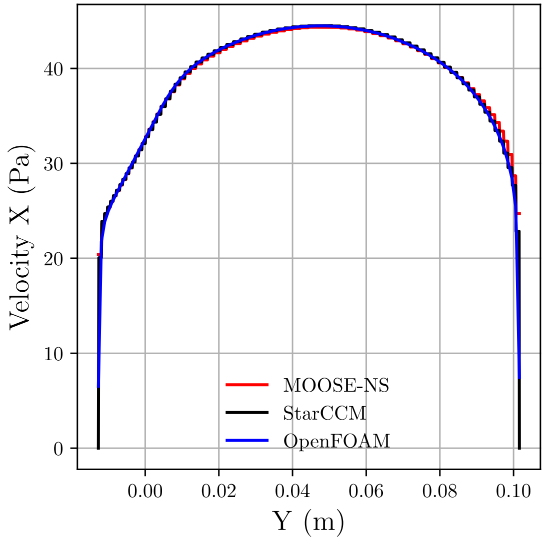
Code-to-code comparison – backward-facing step

- 2D Turbulent flow:
  - Re=36,000
  - Standard k-epsilon model
- Tested with:
  - Star-CCM+
  - OpenFOAM
  - Navier-Stokes module of MOOSE
- Same mesh, same discretization settings
- Comparing:
  - Velocity profiles at the outlet
  - Reattachment length





Velocity profile at outlet

Code	Reattachment length (-)
StarCCM+	4.96
OpenFOAM	5.04
MOOSE-NS	4.76

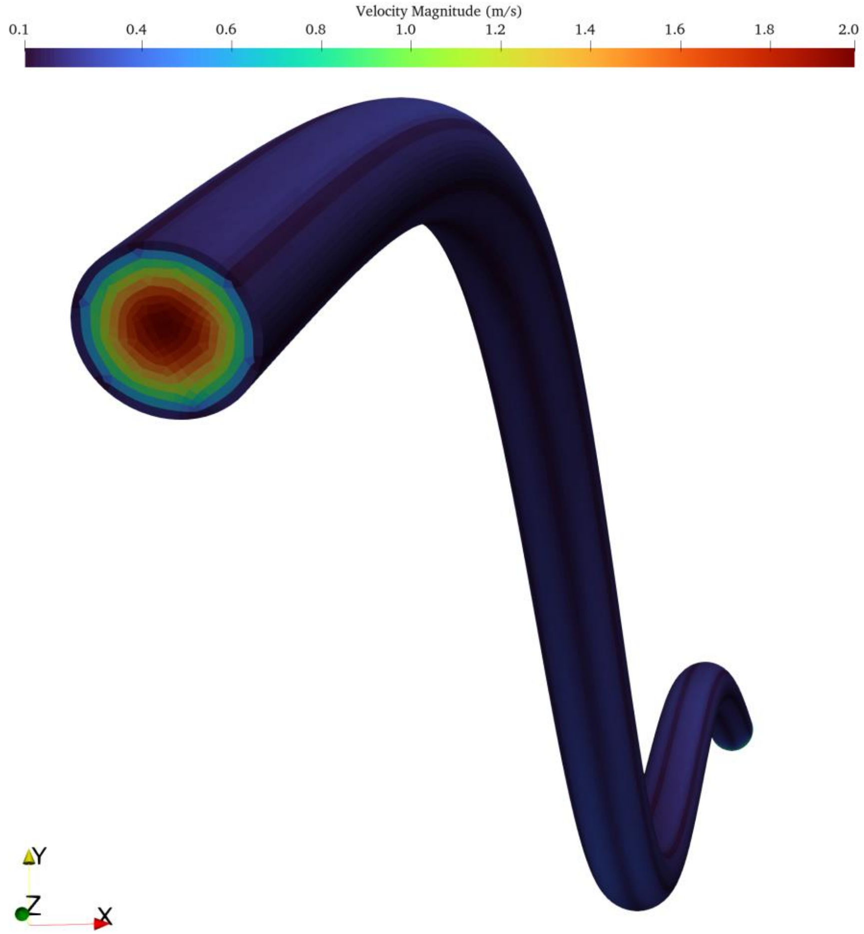
Reattachment length (divided by the step height)

Performance

- 3D wavy pipe case:
  - Laminar flow, Re=100
  - Semi-structured (extruded) mesh with 305k cells
- Target tolerance: 2e-4 (~200 iterations)
- Ran with 48 processes on a desktop machine
- Both segregated approaches are faster than the original monolithic approach
- Results in considerable memory savings as well

Solution algorithm	Runtime (s)	Peak memory usage (GB)
Monolithic, nonlinear FVM	2841 (1x)	134 (1x)
Segregated, nonlinear FVM assembly	671 (~4x)	48 (~0.36x)
Segregated, linear FVM assembly	87 (~33x)	47 (~0.35x)

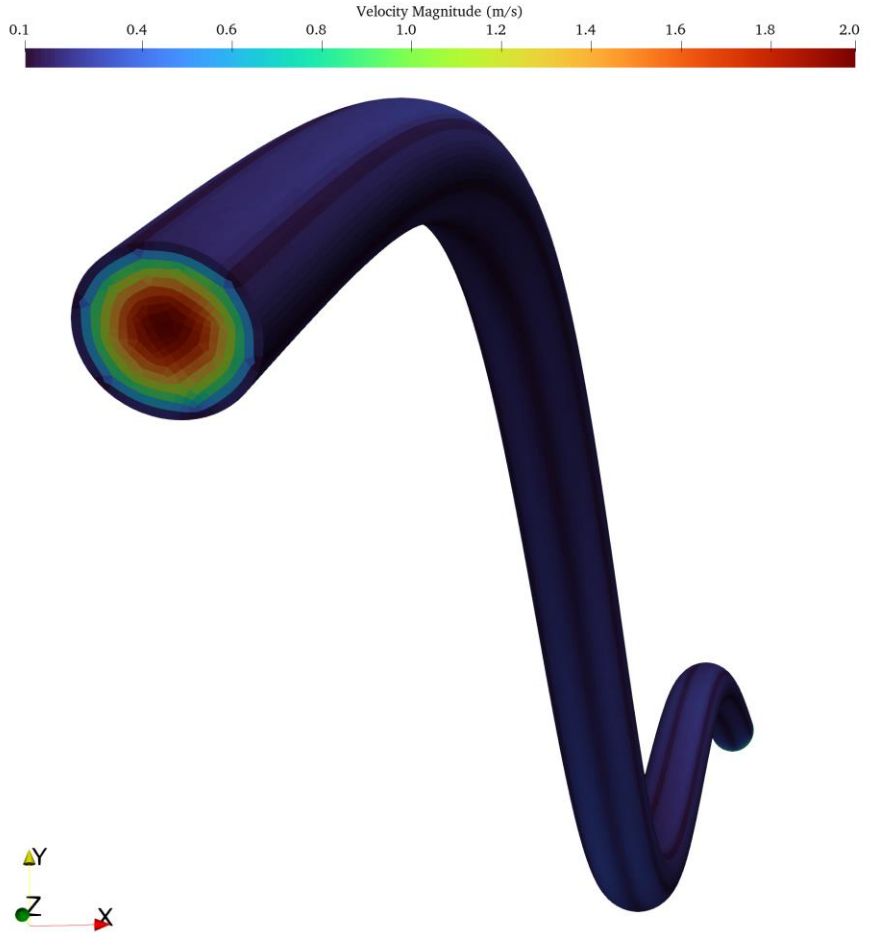
(Speedup and memory reduction compared to initial state is presented in parentheses)



Initial code-to-code performance comparison

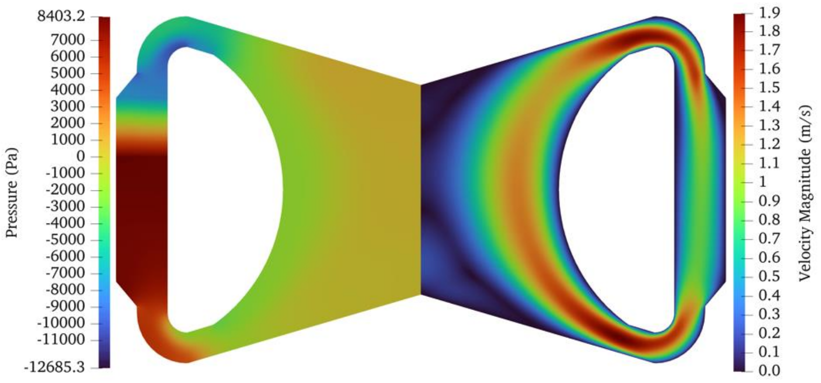
- Ran the same case with:
  - StarCCM+
  - OpenFOAM
  - MOOSE Navier-Stokes module
- All of them used distributed mesh
- Ran with 48 processes on one node of Sawtooth (INL HPC)
- Runtime for this specific case is close to OpenFOAM but still slower than StarCCM+

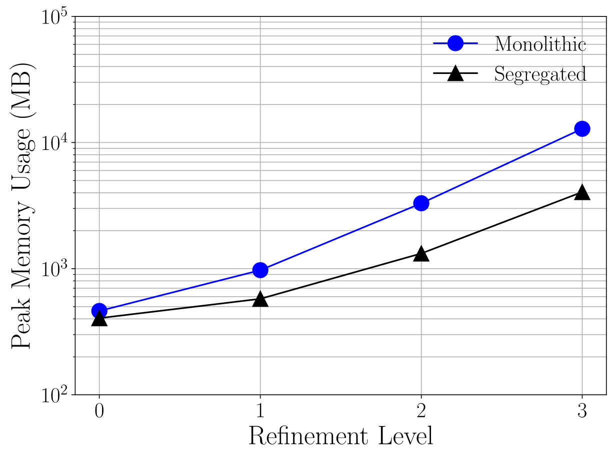
Solver	Runtime (s)
Star-CCM+	19
OpenFOAM	25
MOOSE-NS (with pre-split mesh)	52

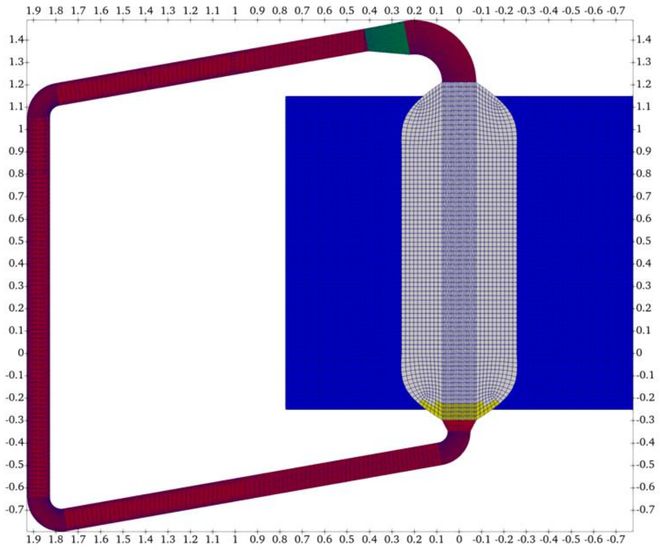


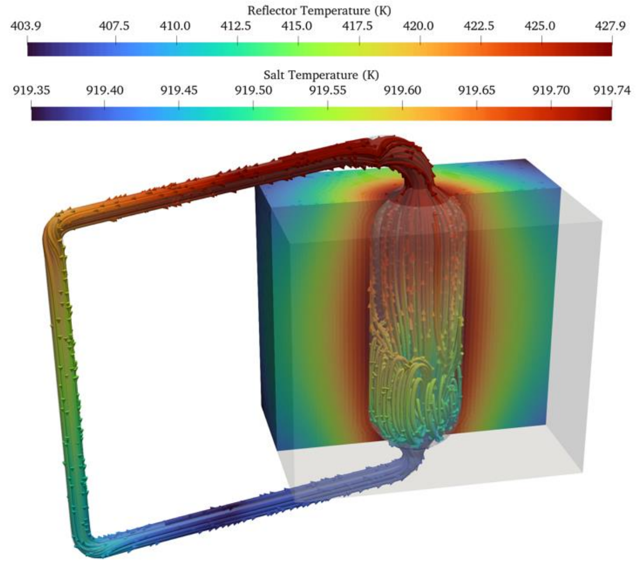
Applications

- Fast spectrum MSRs may have complex flow patterns in the core
- Flow influences neutronics, chemical behavior as well
- Detailed knowledge of the flow field is needed
- Behavior is inherently 3D
- Used to be extremely slow with MOOSE









Ongoing efforts

- Porting functionality to the new segregated solution setting:
  - Enhanced coupling with other MOOSE-based apps (through the MultiApp system)
  - Porous medium corrections
  - Multiphase capabilities
  - Turbulence models
- Employing new capabilities to the confirmatory analysis and engineering of the Molten Chloride Reactor Experiment
- Further extensions for acceleration:
  - SIMPLEC/SIMPLER algorithms for reduced iteration count

Summary

- The SIMPLE algorithm has been implemented in the Navier-Stokes module of MOOSE
- The implementation has been verified using MMS
- The implementation has been validated using some canonical cases both for laminar and turbulent regimes
- More extensive validation is ongoing
- Considerable gains in computational time and memory usage over existing capability

Acknowledgements

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Thank you for your attention!
Questions?