INL/CON-23-75342-Revision-1

The MOOSE fluid properties module

November 2023

Guillaume Louis Giudicelli, Alexander D Lindsay, Benjamin Spaude, Steven Isaacs

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MOOSE Fluid Properties module

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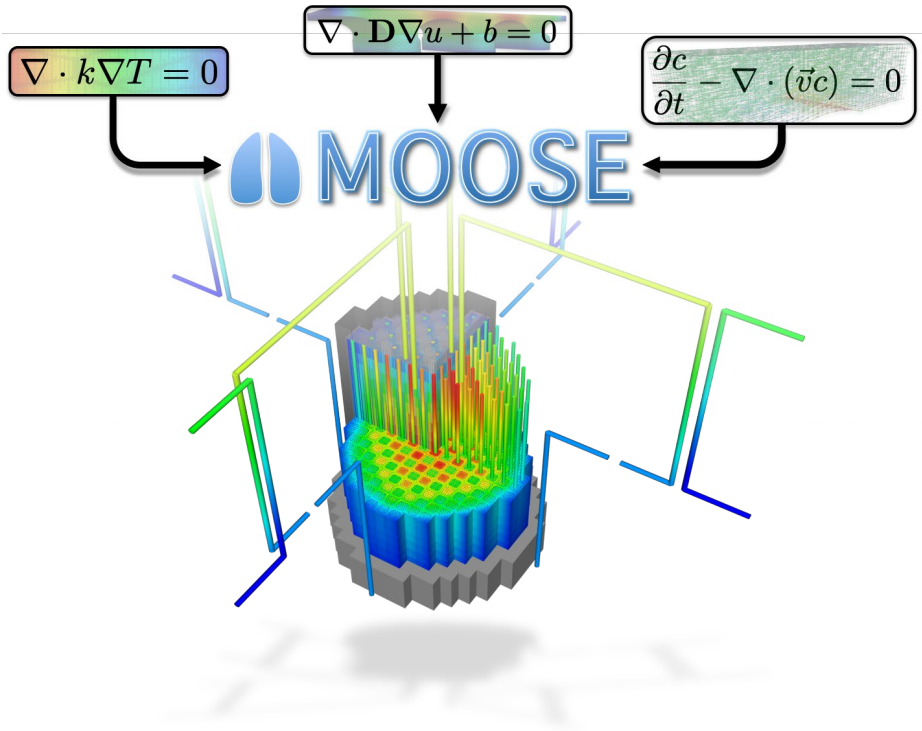
Idaho National Laboratory

Presentation Plan

- MOOSE and the modules
- Applications-driven development
- Features supported
- Fluids supported
- Properties implemented
- Introducing the Solid Properties module

MOOSE: a multiphysics framework

- Multiphysics Object-Oriented Simulation Environment
- Started in May of 2008 (LDRD)
- MOOSE is an object-oriented simulation framework allowing rapid development of new simulation tools
- Code development focuses on implementing physics rather than numerical issues
- Leverages multiple DOE and university-developed scientific computational tools
- Used by multiple national labs, universities, and industry partners
- Ecosystem of diverse applications:
  - Nuclear fuel, reactor physics, geomechanics, mining, chemistry, earthquake prediction, groundwater flow, fluid flow, microstructure evolution, etc.
- Open sourced on March 19, 2014
- Received R&D Award in November 2014.



MOOSE modules

Physics modules

- Heat Transfer
- Mechanics
- Contact
- Phase Field
- Porous Flow
- Navier-Stokes (FE & **FV**)
- Chemical Reactions
- Thermal hydraulics
- Fluid Structure Interaction
- Electromagnetics
- Scalar Transport
- Geochemistry

Numerics modules

- Reconstructed Discontinuous Galerkin
- eXtended Finite Element (XFEM)
- Level Set
- Functional Expansion Tools
- Stochastic Tools
- Ray Tracing
- External petsc solver
- Optimization

Others / Cross-cutting

- Reactor
- **Fluid properties**
- Solid Properties

Applications supported NEAMS

- Pronghorn

Coarse mesh thermal hydraulics for advanced reactor applications

- Pronghorn-Subchannel

Subchannel code for flow in lattices (SFRs, others)

- SAM & RELAP-7

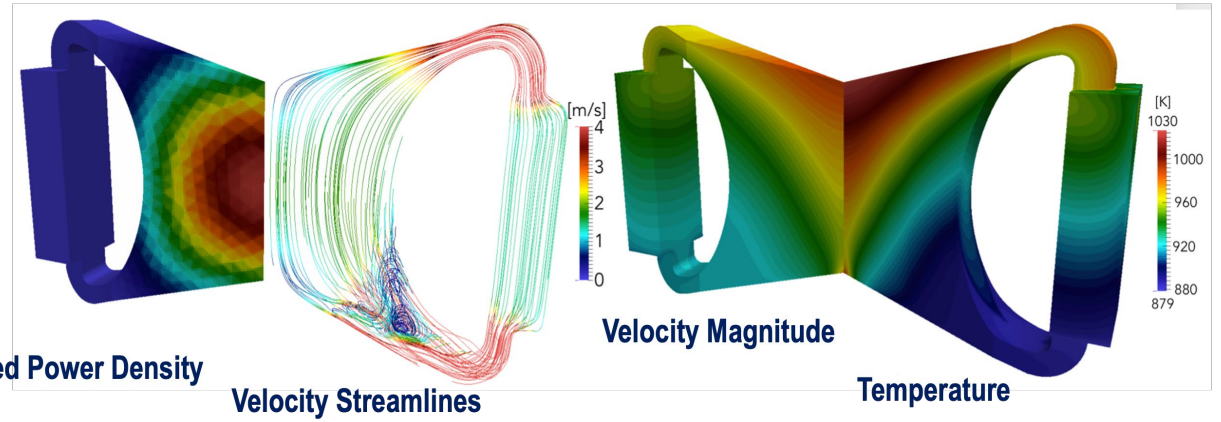
Systems code for advanced reactors

- Sockeye

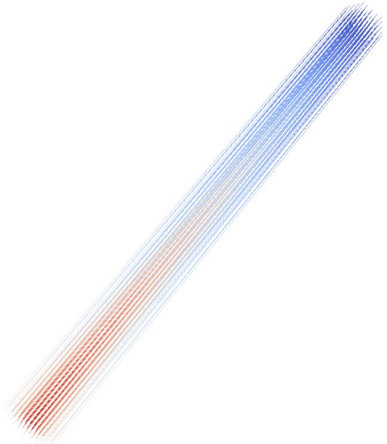
Heat pipe modeling

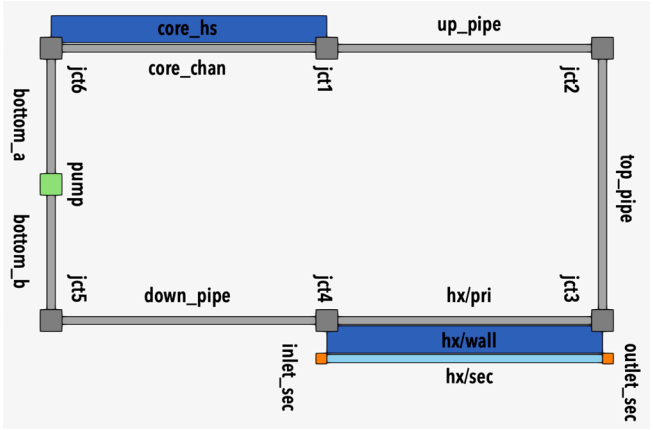
- Cardinal

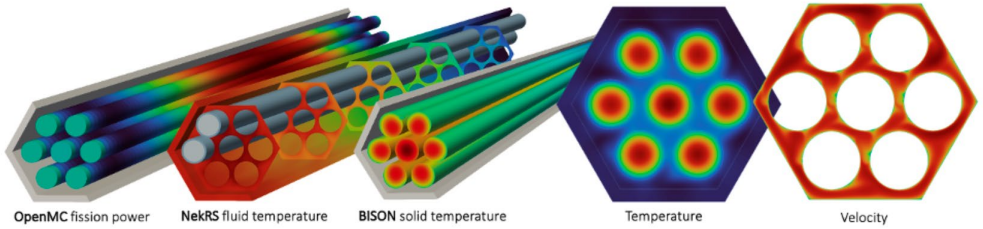
High fidelity multiphysics



Top: Molten salt reactor coarse mesh CFD (Pronghorn) [4]
Right: : Temperature profile in an assembly generated using Subchannel [7]
Bottom left: THM helium loop
Bottom right: Cardinal coupled simulation [8]







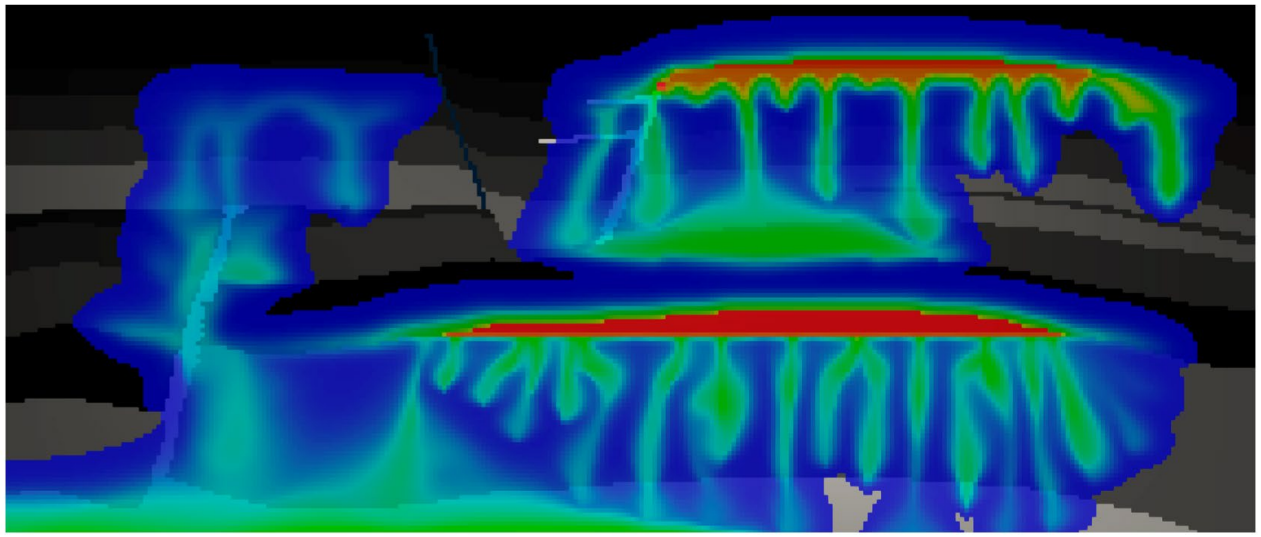
MOOSE Modules supported

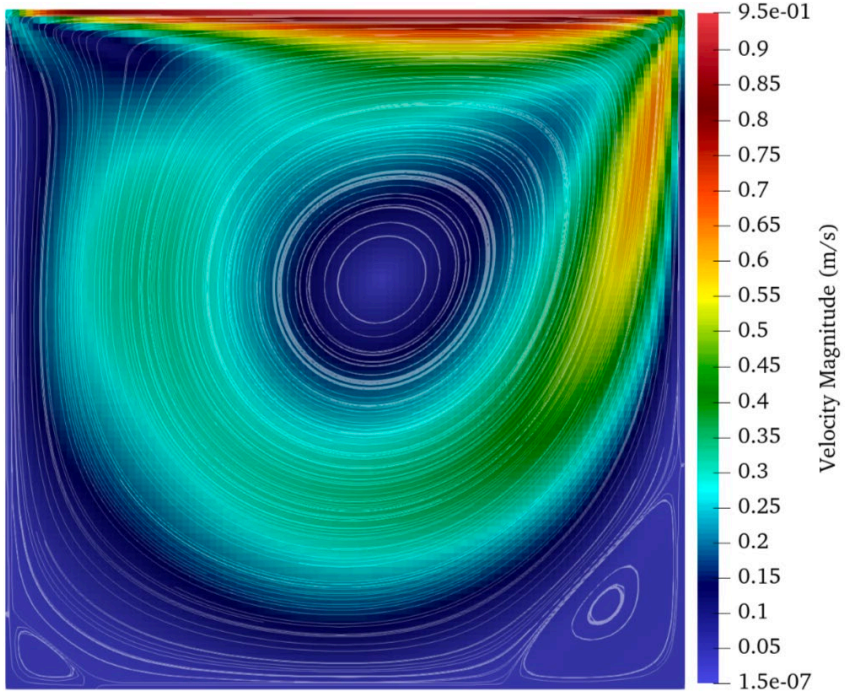
- Porous flow module
- Navier Stokes module

Numerical back-end for Pronghorn

- Thermal hydraulics module

Single-phase thermal hydraulics





Top: Multiphase, multicomponent porous flow simulation of CO2 injection, migration, and dissolution in heterogeneous porous media. CO2 in the gas phase (red) accumulates beneath capillary barriers, and CO2 dissolved in the liquid phase (green) forms convective fingers and sinks to the base. (From Dr. Green CSIRO)
Left: lid driven cavity simulated with Navier Stokes module

Features supported: automatic differentiation

- Module extensively supports automatic differentiation, which lets us compute the derivatives of fluid properties with regards to the nonlinear variables being solved for

TABLE III

Derivative Calculation with Respect to x_1 at $(1, 0.5)$ Using AD*

Function Computation	Derivative Evaluation
$w_1 = x_1 = 1$	$\dot{w}_1 = 1$ (seed)
$w_2 = x_2 = 0.5$	$\dot{w}_2 = 0$ (seed)
$w_3 = \sin(w_2) = 0.48$	$\dot{w}_3 = \cos(w_2) \cdot \dot{w}_2 = 0$
$w_4 = \cos(w_1) = 0.54$	$\dot{w}_4 = -\sin(w_1) \cdot \dot{w}_1 = -0.84$
$w_5 = w_1 w_3 = 0.48$	$\dot{w}_5 = \dot{w}_1 w_3 + w_1 \dot{w}_3 = 0.48$
$w_6 = w_2 w_4 = 0.27$	$\dot{w}_6 = \dot{w}_2 w_4 + w_2 \dot{w}_4 = -0.42$
$w_7 = w_5 + w_6 = 0.75$	$\dot{w}_7 = \dot{w}_5 + \dot{w}_6 = 0.06$

- AD greatly facilitates computation of the exact Jacobian, especially during variable set conversions in which a Newton-Raphson algorithm may be used for the inversion, as it is otherwise difficult to keep track of derivatives during the solve iterations.

Features supported: variable set conversions

(pressure, temperature) used to evaluate properties for incompressible / weakly compressible flow equations formulations

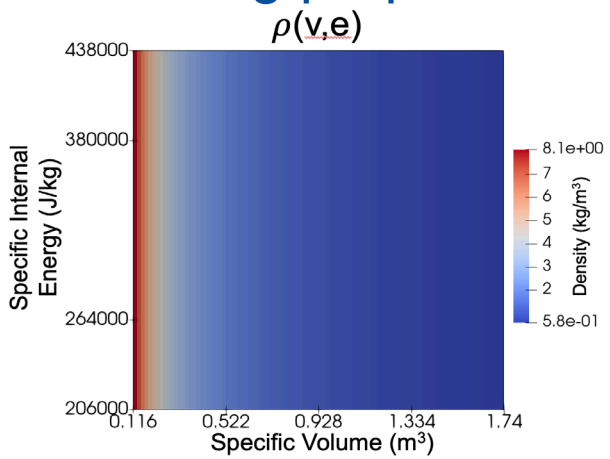
(specific volume, specific internal energy) for evaluating properties for compressible flow formulations

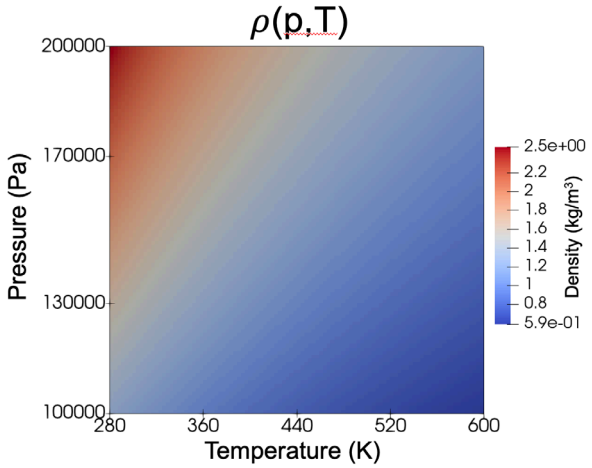
Conversions:

Newton 1D and 2D solves, with AD:

$$\text{Find T such that: } \rho(T) = \rho_0$$

$$\text{Find p, T such that: } \rho(p,T) = \rho_0$$
$$e(p,T) = e_0$$





Features supported: automated out-of-bounds checking

- Correlations have ranges of validity due to the limited range of measurements, to physical phenomena (boiling, solidification), etc

```
Real
NaKFluidProperties::rho_from_p_T(Real /*pressure*/, Real temperature) const
{
  const Real Tc = temperature - _T_c2k;
  // Range from liquid Na and K density correlation ranges
  if (Tc < 210 || Tc > 1110)
    flagInvalidSolution(
        "NaK density evaluated outside of Na density temperature range [210, 1110] C");
  if (Tc < 63.2 || Tc > 1250)
    flagInvalidSolution(
        "NaK density evaluated outside of K density temperature range [63, 1250] C");
```

- Fluid properties can accidentally be evaluated out of bounds

- Two simple interfaces

- NaNInterface

- SolutionInvalidInterface

```
Real
IdealGasFluidProperties::p_from_v_e(Real v, Real e) const
{
  if (v <= 0.0)
    return getNaN("Invalid value of specific volume detected (v = " + Moose::stringify(v) + ").");

  return (_gamma - 1.0) * e / v;
}
```

Fluids implemented

Categories:

General form
- tabulated
- functionalized

Gas models
- ideal gas
- stiffened gas
…

Advanced reactor coolants
- Gases
- liquid metals
- molten salts

Two phase models
Mixture models

Table II: Summary of fluid properties classes available in the module, the variable sets implemented, and the general compatibility with MOOSE modules. (Most fluid properties classes are suffixed with `FluidProperties`, which is omitted here for brevity.)

Fluid	(p,T)	(v,e)	Navier-Stokes	Thermal Hydraulics	Subchannel	Porous Flow
Single-phase						
Brine [28,36–38]	yes	yes	no	no	N/A	yes
Air (ideal gas)	yes	yes	yes	yes	yes	yes
CO_2 [39]	yes	no	no	no	no	yes
StiffenedGas	yes	yes	yes	yes	yes	yes
CaloricallyImperfectGas	yes	yes	yes	yes	no	yes
Helium [40]	yes	yes	yes	yes	yes	yes
Hydrogen [41,42]	yes	no	no	no	no	yes
Methane [43]	yes	no	no	no	no	yes
Halite - NaCl [29]	yes	no	yes	no	no	no
Nitrogen [44]	yes	no	no	no	no	yes
SodiumSaturation [32]	yes	no	yes	no	no	N/A
Water IAPWS-IF97 [26,27]	yes	yes	yes	yes	no	yes
Simple (exponential density)	yes	yes	yes	yes	yes	yes
Linear (linear density in p,T)	yes	yes	yes	yes	no	no
Tabulated	yes	yes	yes	yes	no	yes
FLiBe salt [31]	yes	no	yes	no	yes	N/A
FLiNaK salt [31]	yes	no	yes	no	yes	N/A
Lead [35]	yes	no	yes	no	yes	N/A
Lead Bismuth [35]	yes	no	yes	no	yes	N/A
NaK eutectic [34]	yes	no	yes	no	yes	N/A
Two-phase						
TwoPhaseIndependent	no	yes	no	no	no	no
TwoPhaseNonCompressibleGas	no	yes	no	no	no	no
StiffenedGasTwoPhase	no	yes	no	no	no	no
Vapor mixtures						
IdealRealGasMixture	yes	yes	no	no	no	no

Properties implemented in the module

Table I: Summary of the thermophysical properties available for single-phase fluids in the Fluid Properties module, and the variable sets implemented

Variable set	(p,T)	(v,e)	(h,s)	(p,s)	(h,p)	(ρ,T)	(p,ρ)
pressure (p)	-	yes	yes	-	-	yes	-
temperature (T)	-	yes	no	no	yes	-	no
density (ρ)	yes	-	no	yes	no	-	-
dynamic viscosity (μ)	yes	yes	no	no	no	yes	no
thermal diffusivity (k)	yes	yes	no	no	no	yes	no
speed of sound (c)	yes	yes	no	no	no	no	no
isobaric heat capacity (c_p)	yes	yes	no	no	no	no	no
isochoric heat capacity (c_v)	yes	yes	no	no	no	yes	no
specific internal energy (e)	yes	-	no	no	no	yes	yes
specific enthalpy (h)	yes	yes	-	no	-	yes	no
specific entropy (s)	yes	yes	-	-	yes	yes	no
specific free energy (g)	no	yes	no	no	no	no	no
thermal expansion coeff. (β)	yes	no	no	no	no	no	no
c_p/c_v (γ)	yes	yes	no	no	no	no	no

Rigorous testing

- Properties are all tested using unit tests
- Testing occurs on all pull requests made to MOOSE, and all releases
- Code coverage of 84%, on an upwards trend
- Unit testing includes:
  - Value checks (regression testing) at values over the domain of definition
  - Derivatives checks using finite differencing
  - Consistency checks between (p, T) and (v, e)

    For example, check:

    $h(p, T) = h(v(p,T), e(p,T))$
  - Exception checks to check the error/out-of-bounds behavior

Introducing the Solid Properties module

- Follows the same format as the Fluid Properties module
- To support BISON and MOOSE mechanics calculations

- Contains thermal properties for:

- Graphite grade H_451
- Composite and monolithic SiC
- Stainless steel 316

- We would welcome contributions of standalone properties
  - Only requires a basic understanding of C++ and thermo-dynamics
  - Use OECD/NEA/DOE/.. technical reports as references for the ‘right’ correlations

References

- [1] .Cody J. Permann and Derek R. Gaston and David Andrs and Robert W. Carlsen and Fande
- Kong and Alexander D. Lindsay and Jason M. Miller and John W. Peterson and Andrew E. Slaughter and Roy H. Stogner and Richard C. Martineau. {MOOSE}: Enabling massively parallel multiphysics simulation, 2022, SoftwareX, http://www.sciencedirect.com/science/article/pii/S2352711019302973
- [2] . Fazio, et al., I.S. (2015). Handbook on Lead-bismuth Eutectic Alloy and Lead Properties, Materials Compatibility, Thermal-hydraulics and Technologies- 2015 Edition (NEA--7268). Nuclear Energy Agency of the OECD (NEA)
- [3] "Infographic: How Does Nuclear Thermal Propulsion Work?" *Energy.gov*, https://www.energy.gov/ne/downloads/infographic-how-does-nuclear-thermal-propulsion-work.
- [4] Figure made by Mauricio Tano using the MOOSE Navier Stokes module
- [5] Pioro, Igor, Mokry, Sarah. "Thermophysical Properties at Critical and Supercritical Pressures". Heat Transfer - Theoretical Analysis, Experimental Investigations and Industrial Systems, edited by Aziz Belmiloudi, IntechOpen, 2011. 10.5772/13790.
- 6 RELAP-7 Theory Manual, INL/EXT-14-31366 (Revision 2)
- 7 Development of a Subchannel Capability for Liquid-Metal Fast Reactors in Pronghorn, Tano et al., INL/EXT-22 (in processing)
- 8 MOOSE Fluid Properties Module paper, to be published

Takeaways

- The fluid properties module in MOOSE is an open-source implementation of fluid properties
  - Covers numerous flow applications, tied or not to Nuclear Energy
  - Several functionalized formulations for maximum flexibility
  - Easily extendable
- Recent releases:
  - the extension of TabulatedFP to conserved variable set (v,e)
  - NaK eutectic
  - Lead and Lead Bismuth
  - General functions user input of pressure, temperature
- Work in progress: linking to Saline
- Acknowledgements:

DOE NEAMS Program

DOE SULI internship program

ANL LDRD Program

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