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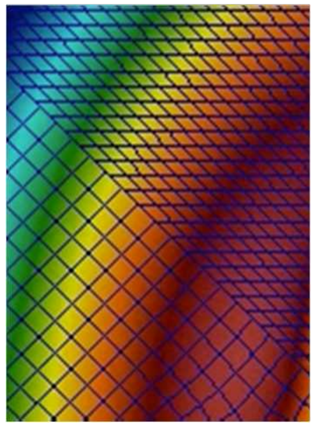

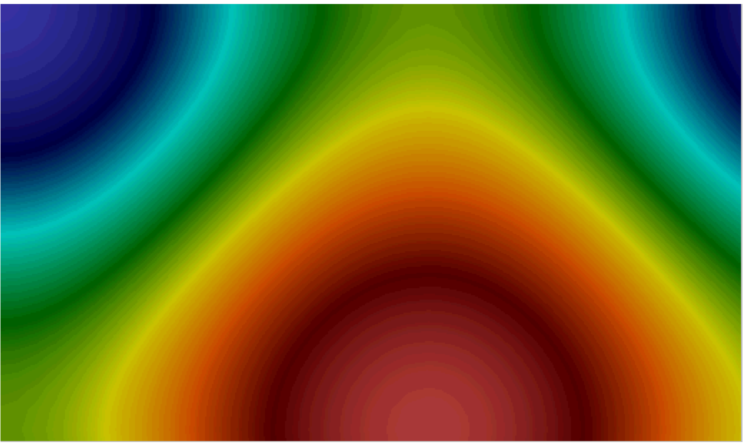

# An Overview of Sierra Mechanics as Applied to Multiphysics Problems with a Detailed Study into the Nonlinear Behavior of a Coupled Piston–Fluid System

**Jonathan Clausen**

Sandia National Laboratories

Albuquerque, NM

*Exceptional service in the national interest*

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**SAND2016-5261 C**

# Outline

- Sierra Mechanics
- Piston–fluid system
- Next-generation platforms


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Mario Martinez
Bill Erikson
John Torczynski
Christian Trott
Rekha Rao

# Sierra Mechanics

Sandia National Laboratories

COMPSIM

Sierra an engineering mechanics simulation code suite supporting the Nation’s Nuclear Weapons mission, as well as other customers.

# Sierra Mechanics



COMPSIM

COMPSIM
THERMAL FLUIDS

COMPSIM
SOLID MECHANICS

COMPSIM
STRUCTURAL DYNAMICS

COMPSIM
VERIFICATION & VALIDATION

COMPSIM
MESHING

COMPSIM
TOOLKIT

# Thermal Fluids



COMPSIM
THERMAL FLUIDS

Fuego

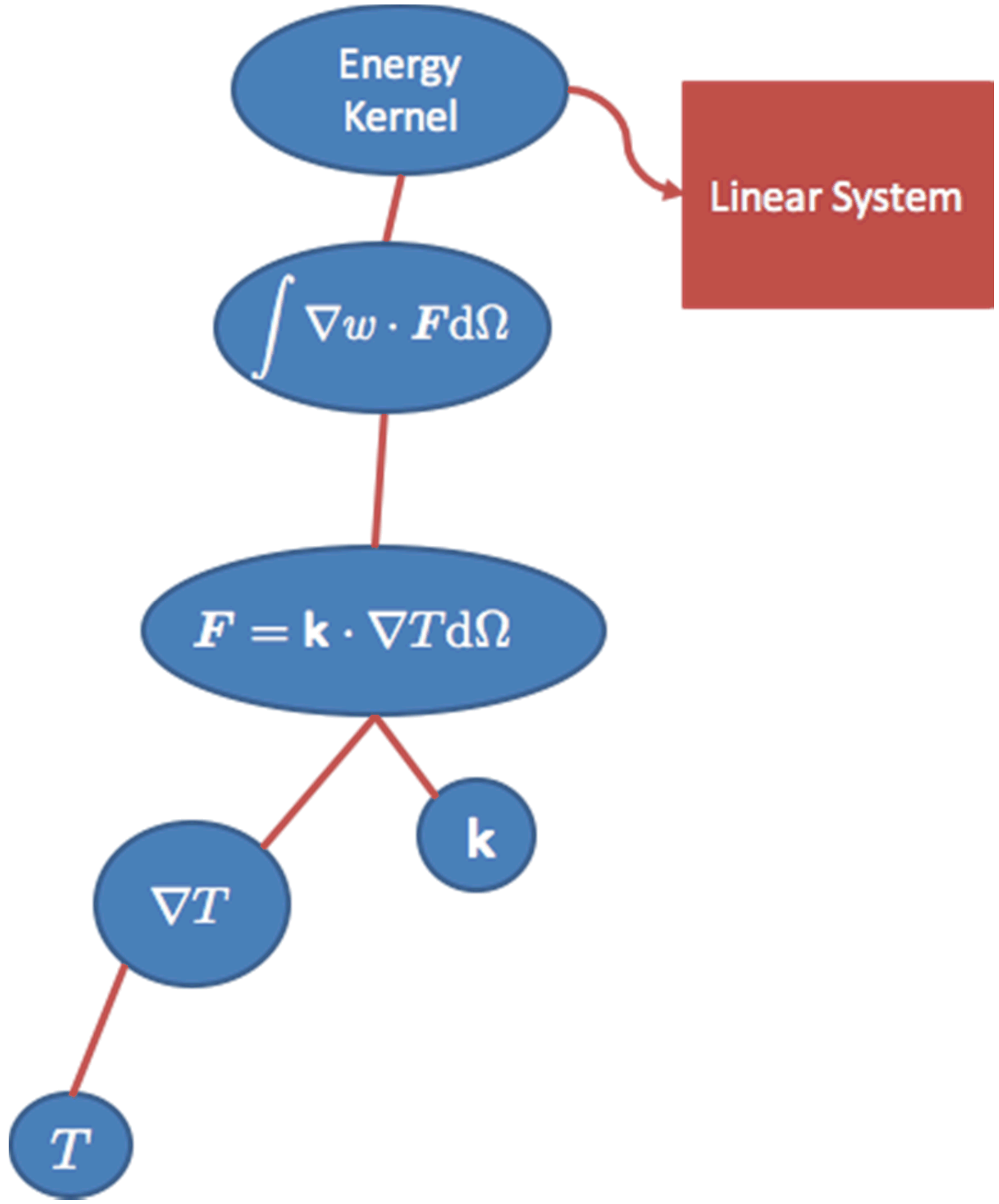
Aero

Nalu

Aria

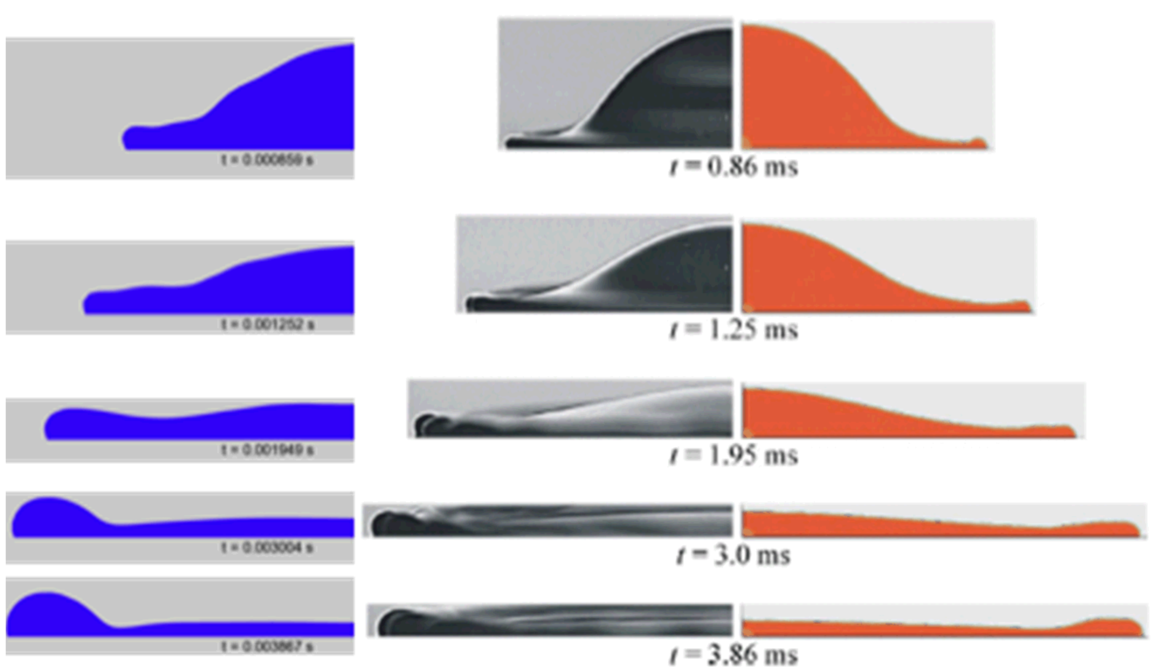
# Aria

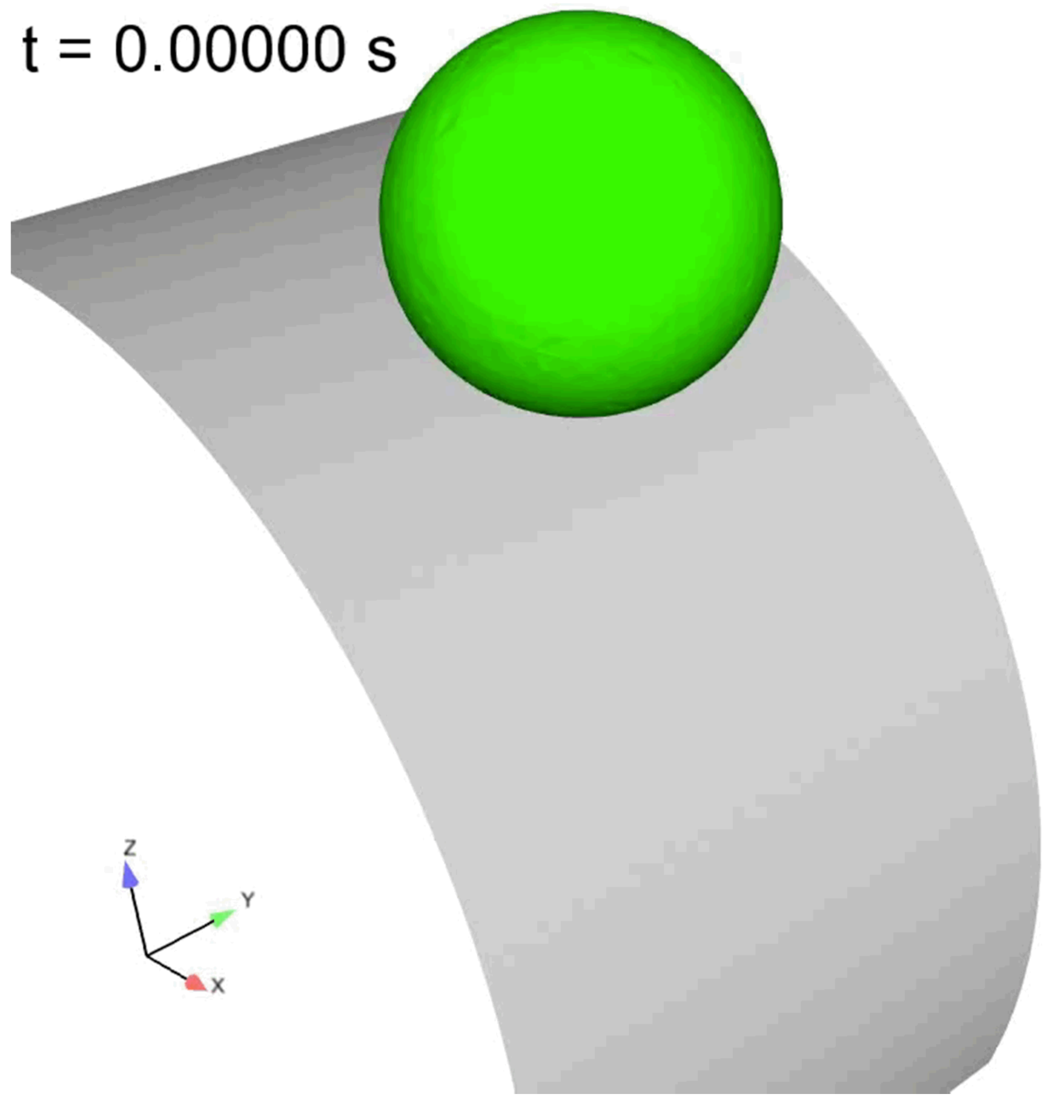
- nonlinear finite element
- stabilized Galerkin (Q1, Q2, P0)
- full Newton sensitivities
- solvers (Trilinos)
- MPI
- monolithic or segregated coupling
- many equations (energy, mass, momentum, species transport, generalized chemistry, voltage)
- expression based



# Aria: Drop impact

- microscale drops impact solid surfaces
- physics
  - fluid dynamics
  - interfacial dynamics
  - energy transport

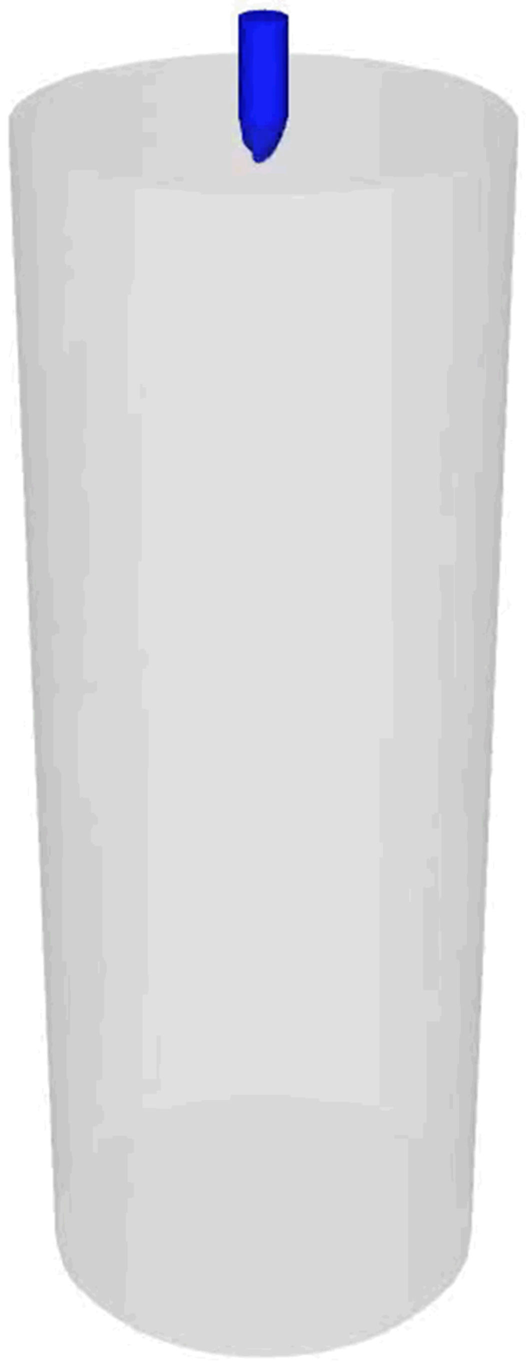



S. Roberts

# Aria: Bottle filling

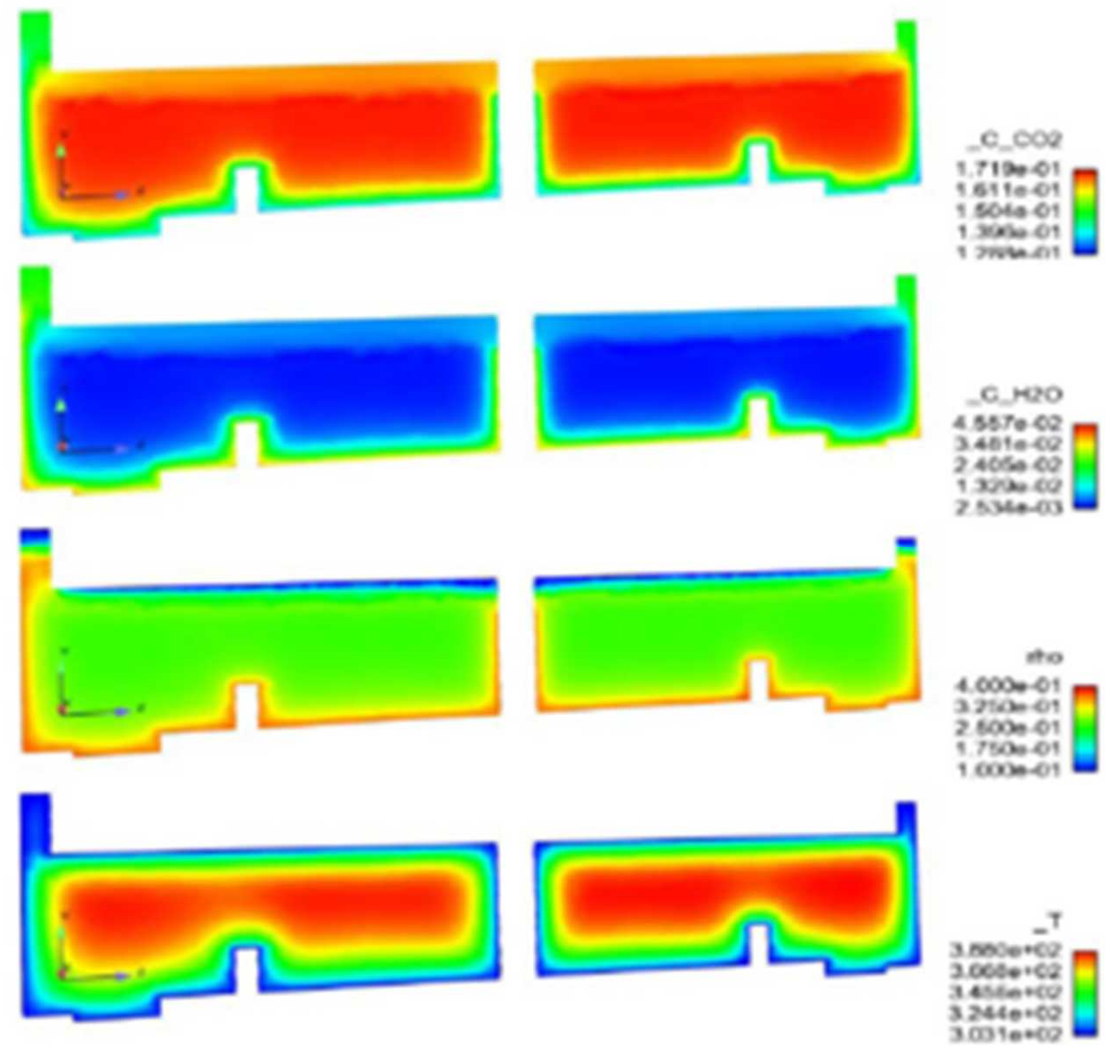
- filling on complex-shaped bottles with non-Newtonian fluids
- physics
  - fluid dynamics
  - mutliphase flow
  - complex constitutive models

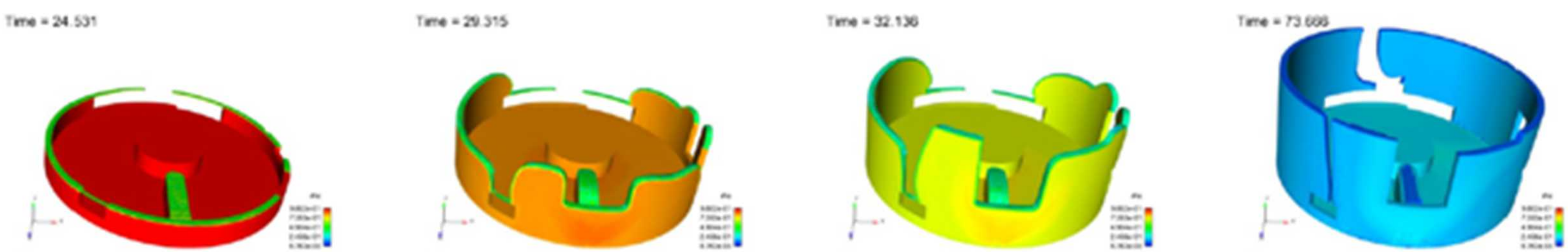


S. Roberts

# Aria: Mold filling with reacting foams

- filling detailed molds with reacting encapsulating foams
- physics
  - fluid dynamics
  - heat generation and transport
  - foam reaction and species transport
  - complex geometry
- design of mold shapes and vent locations for even filling

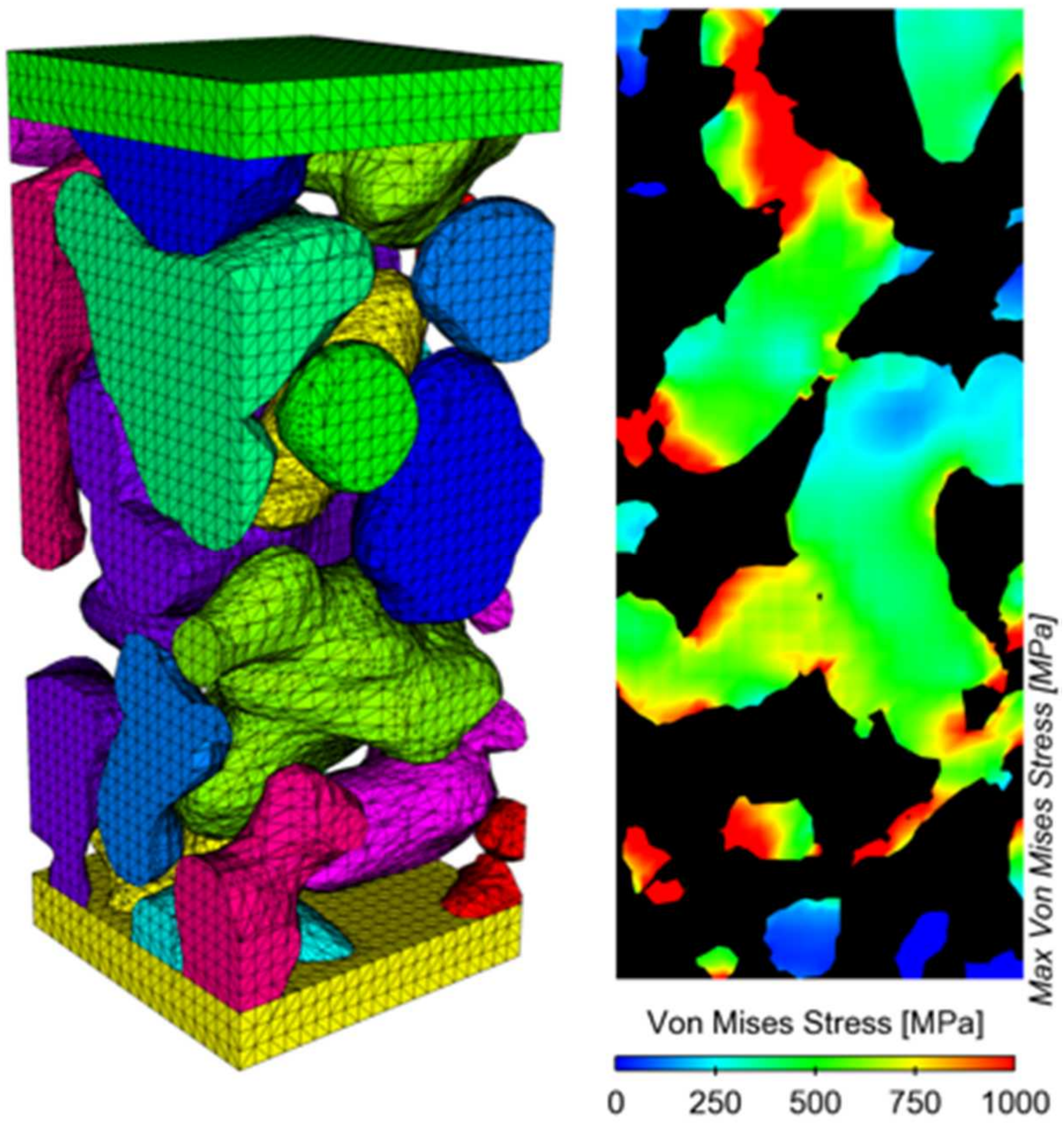


R. Rao

# Aria: Mesoscale modeling of Li-Ion Battery

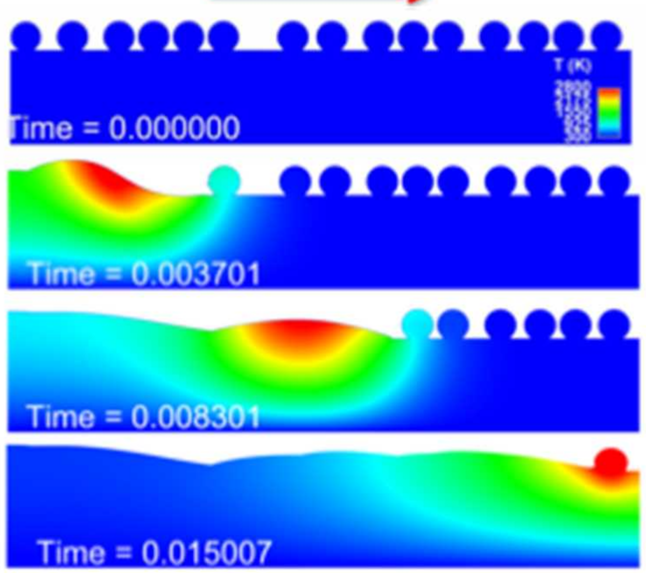
- realistic microstructures
- physics
  - electrochemistry
  - solid mechanics
- motivation
  - understand electrochemistry battery performance
  - study deformation of constituent particles under electrochemical forces
  - identify damage to materials



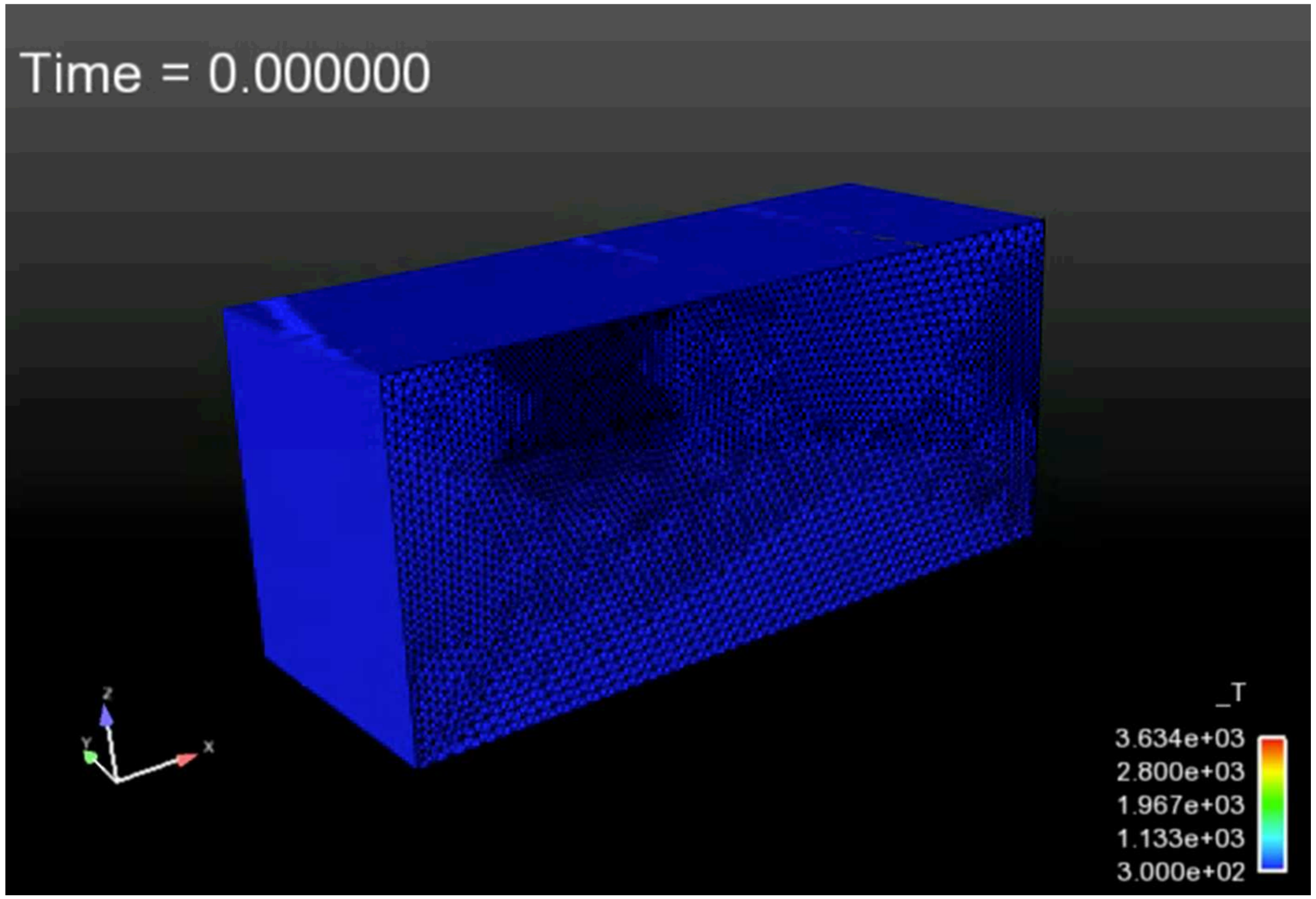

S. Roberts, H. Mendoza, V. Brunini

# Aria: Laser Welding

- laser welding and additive manufacturing via selective laser melting
- physics
  - laser heating
  - nonequilibrium vaporization
  - conduction
  - capillary forces



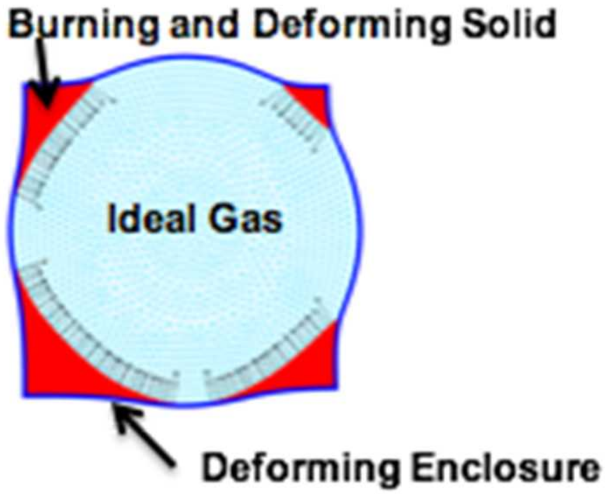

Additive Manufacturing via selective laser melting

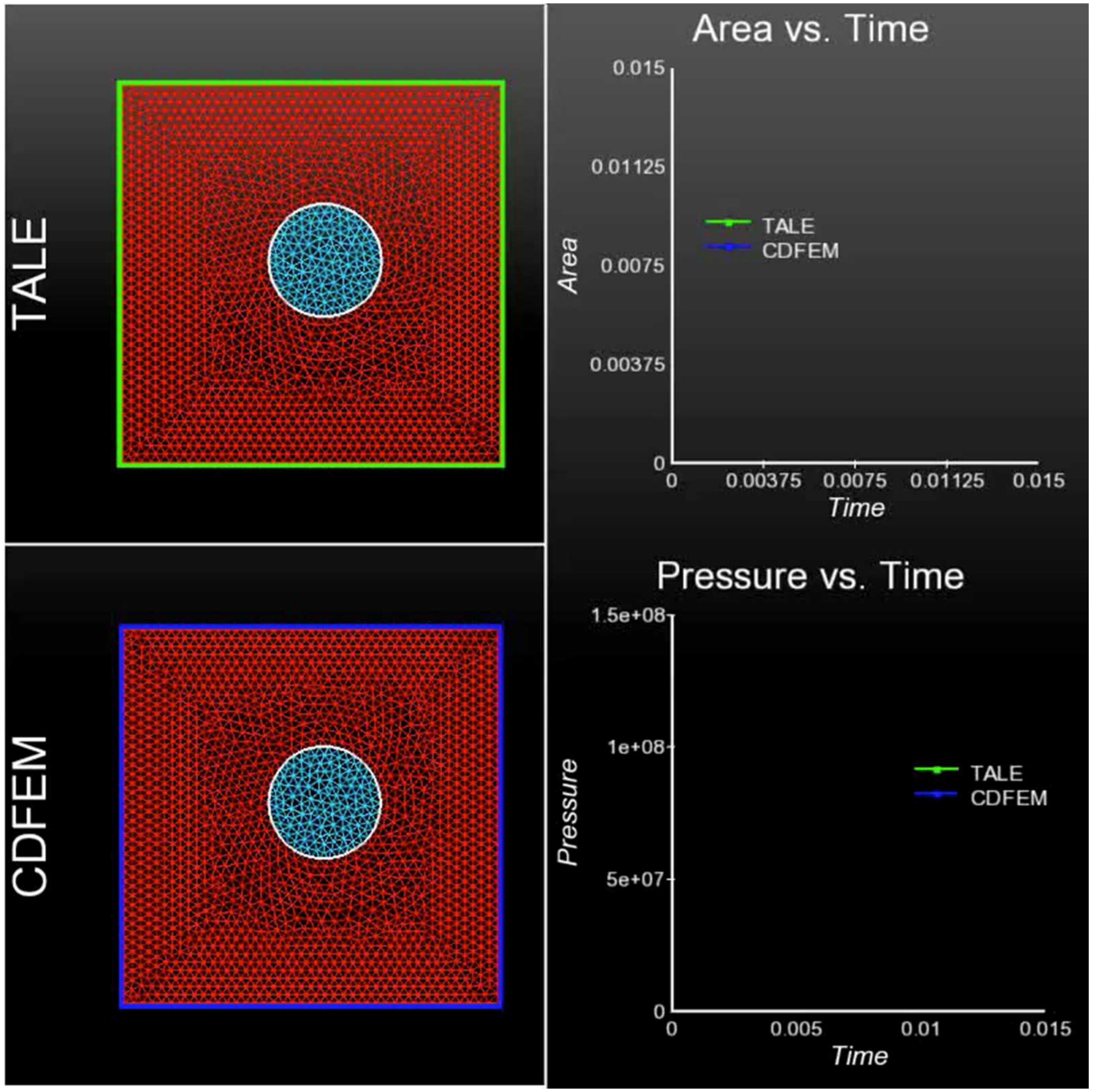



D. Noble, M. Martinez

# Aria: Burning deformable solid

- model burning of energetic material
- physics
  - 3 disparate materials and physics
  - discontinuous DOFs
  - mass/momentum balances
  - burnt front velocity
  - dynamic topology



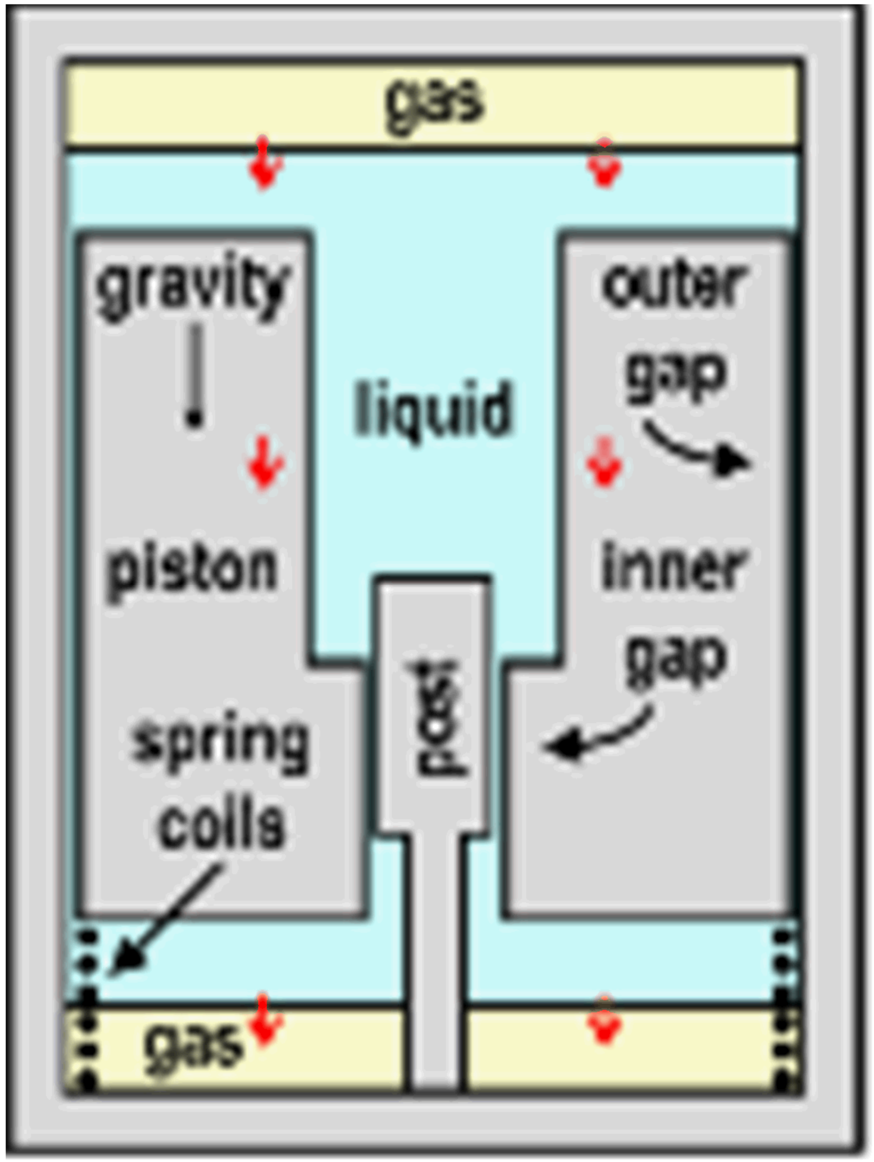




D. Noble, B. Erikson

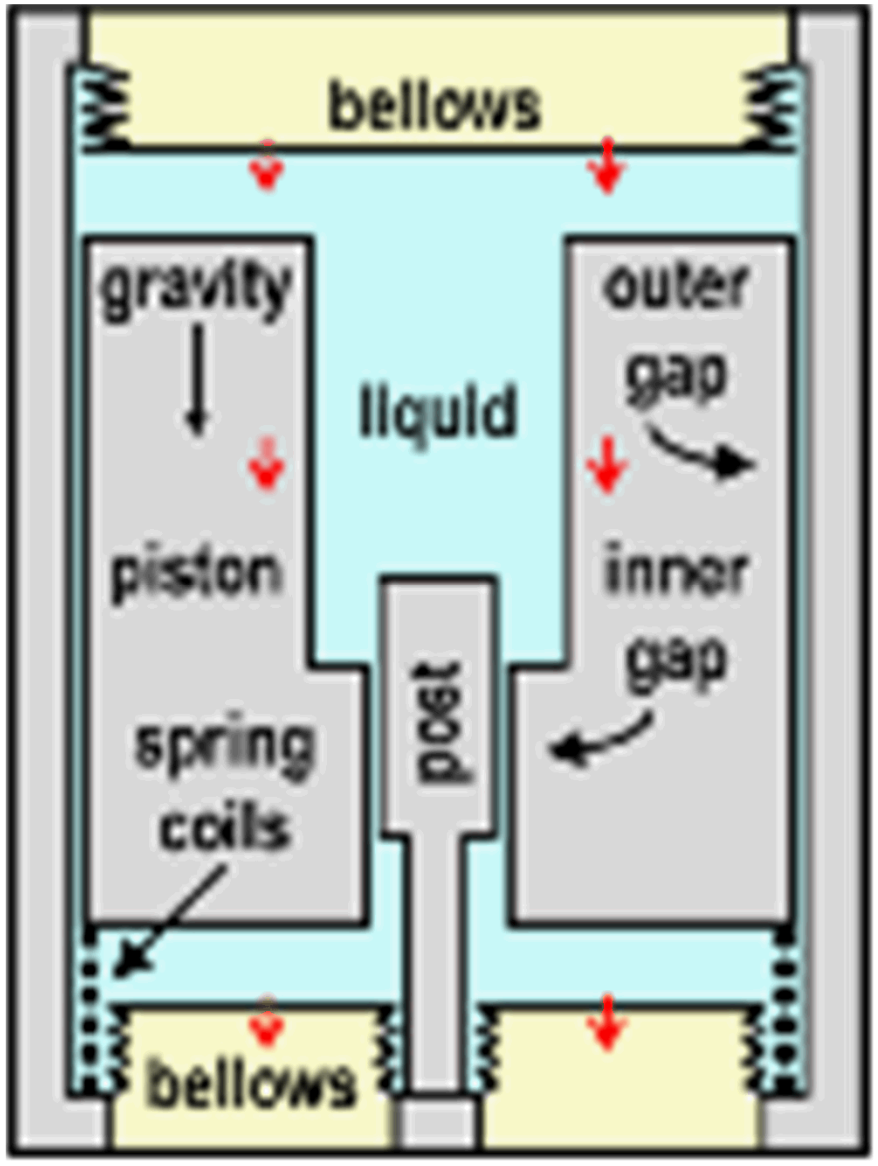
# Outline

- Sierra Mechanics
- **Piston–fluid system**
- Next-generation platforms

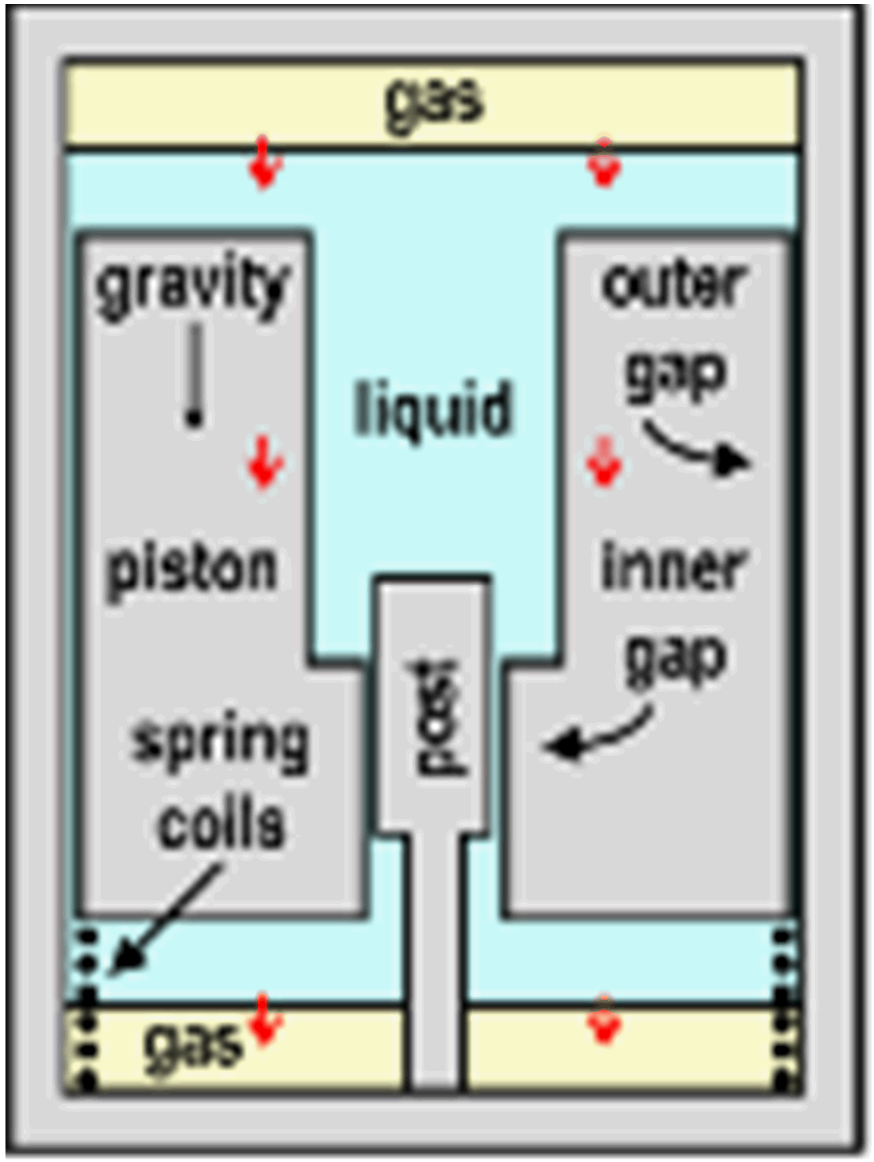
# Motivation


gas
gravity
liquid
outer gap
piston
inner gap
post
spring coils
gas

# Motivation



bellows
gravity
liquid
outer
gap
piston
inner
gap
post
spring
coils
bellows

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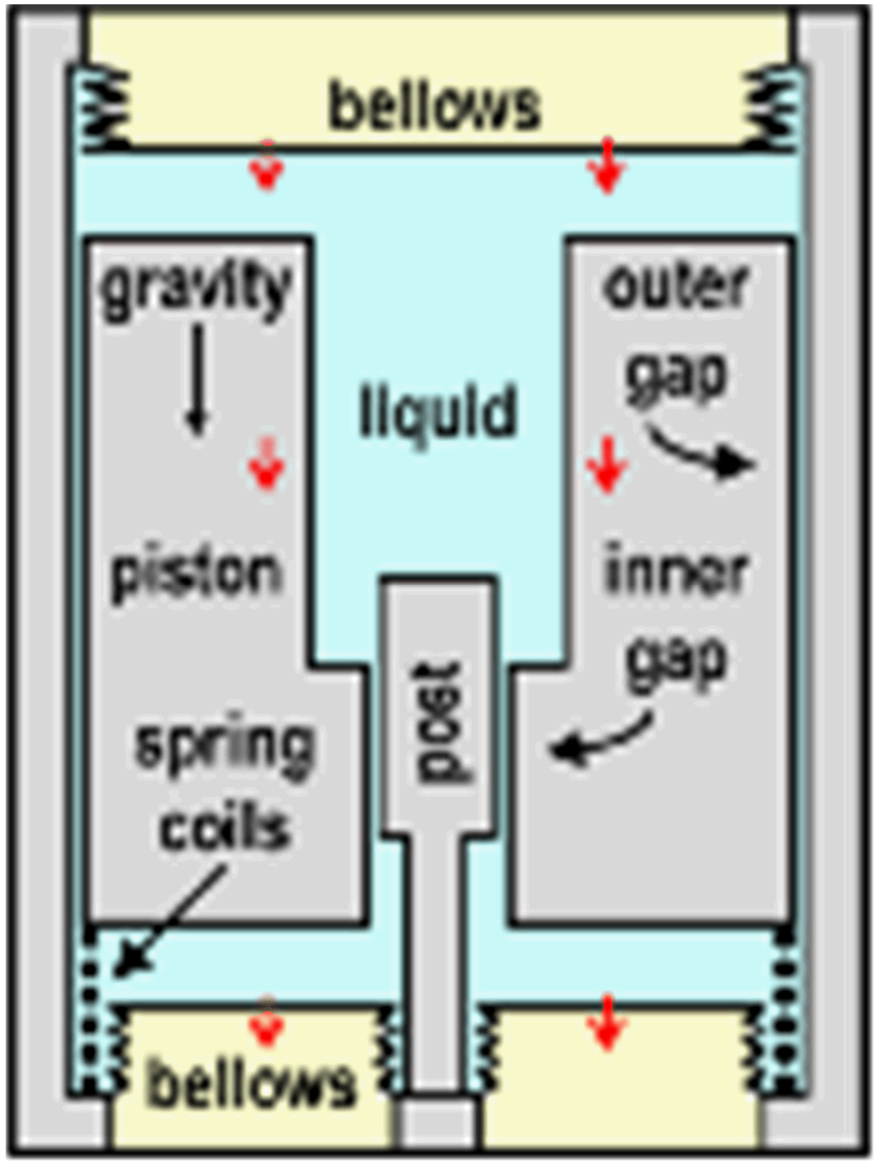

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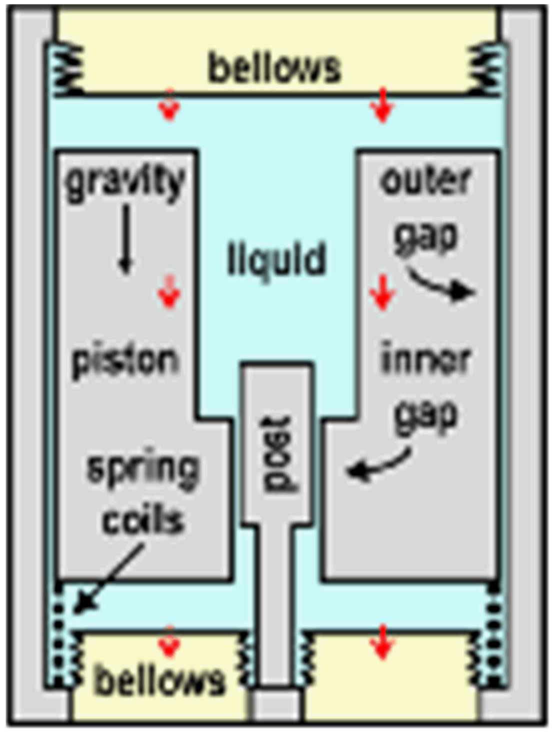
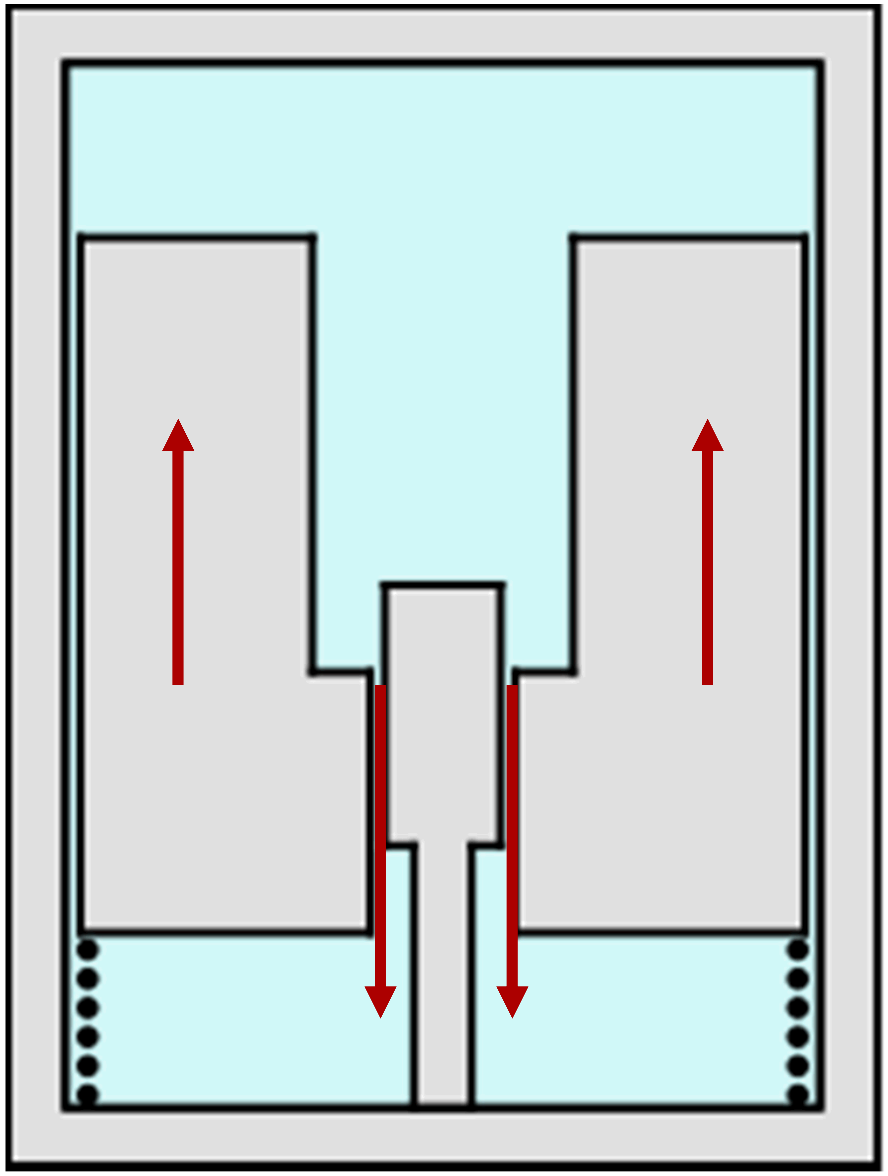
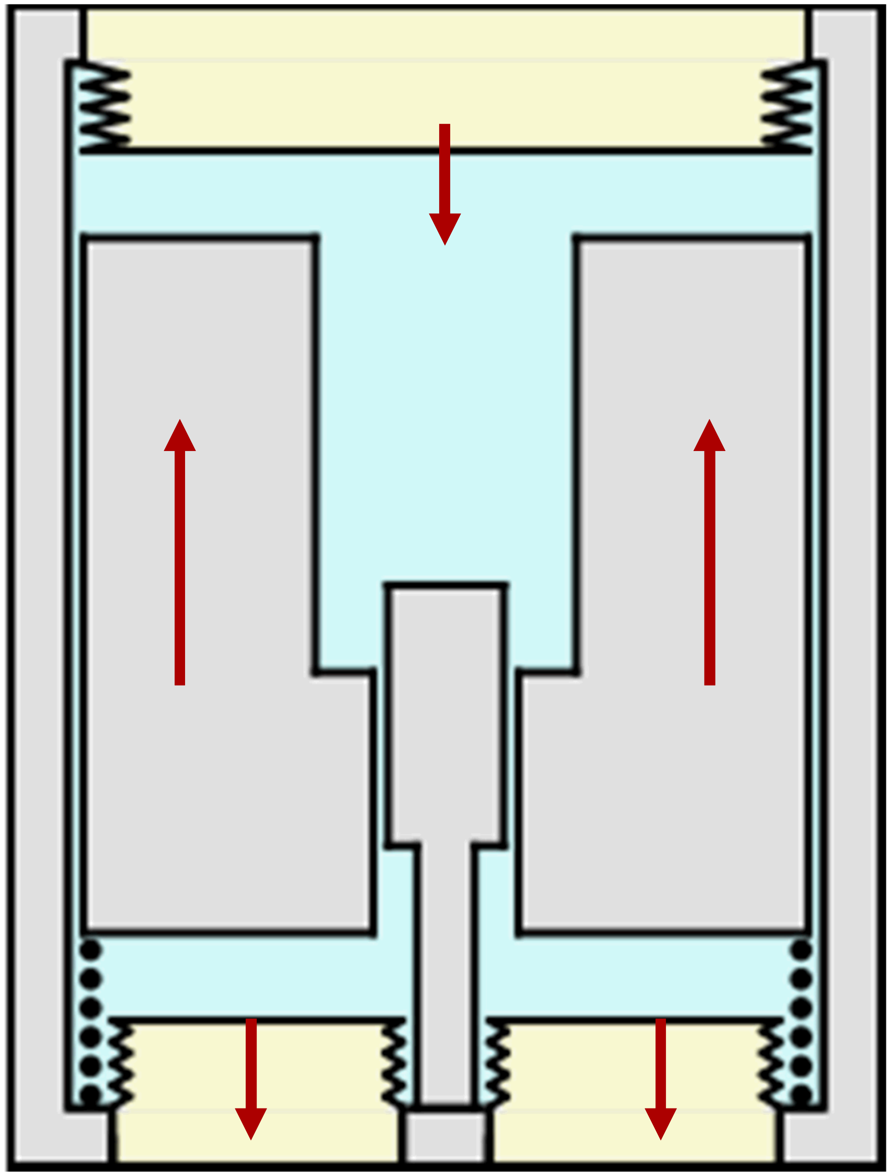
# Motivation



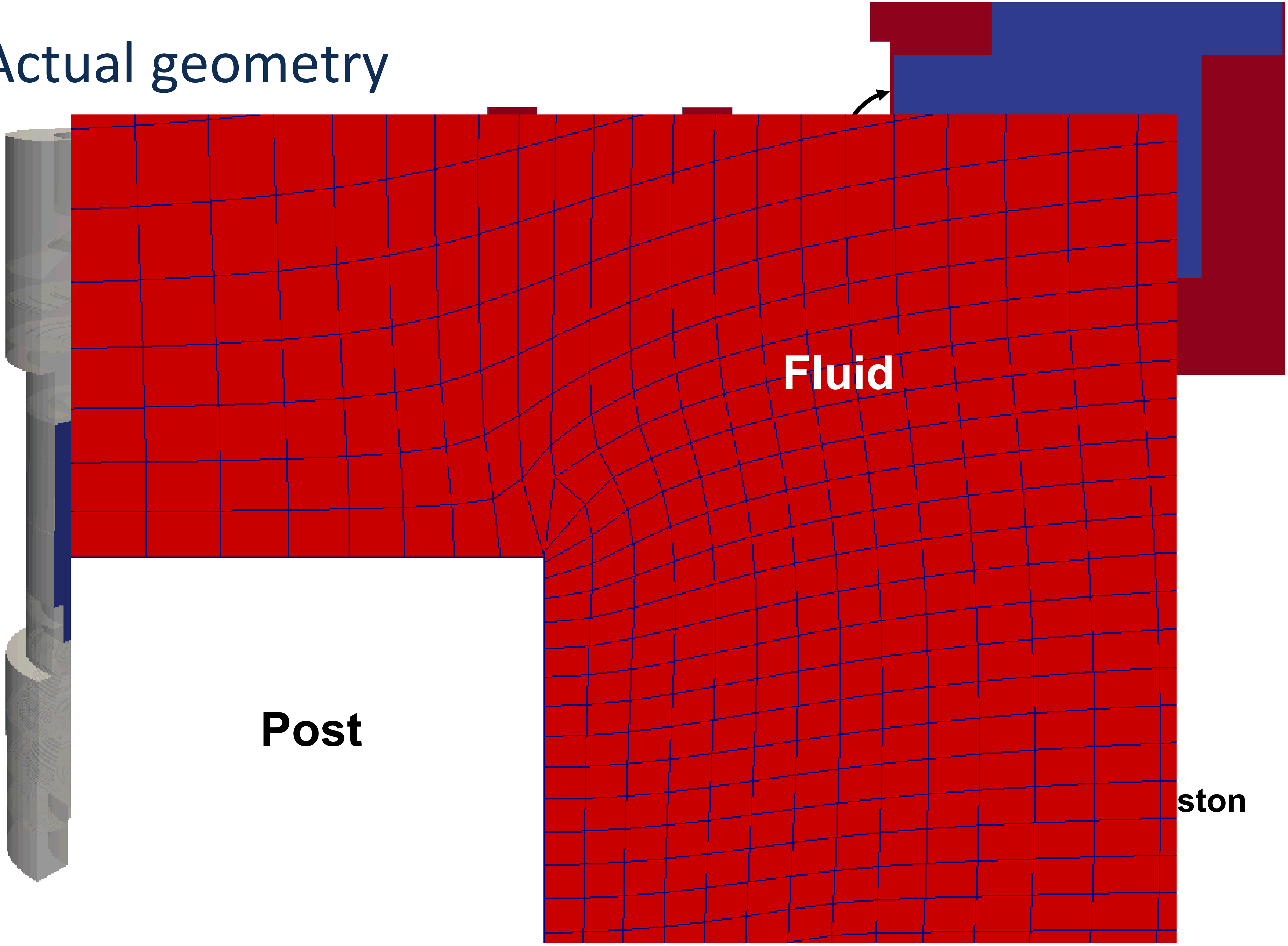

Poiseuille Mode



Couette Mode



# Actual geometry



# Finite-Element Problem Statement

**Strong Form**

$$\nabla \cdot \boldsymbol{u} = 0$$

$$\rho \frac{\partial \boldsymbol{u}}{\partial t} + \rho \boldsymbol{u} \cdot \nabla \boldsymbol{u} = \nabla \cdot \boldsymbol{\sigma} + \boldsymbol{S}$$

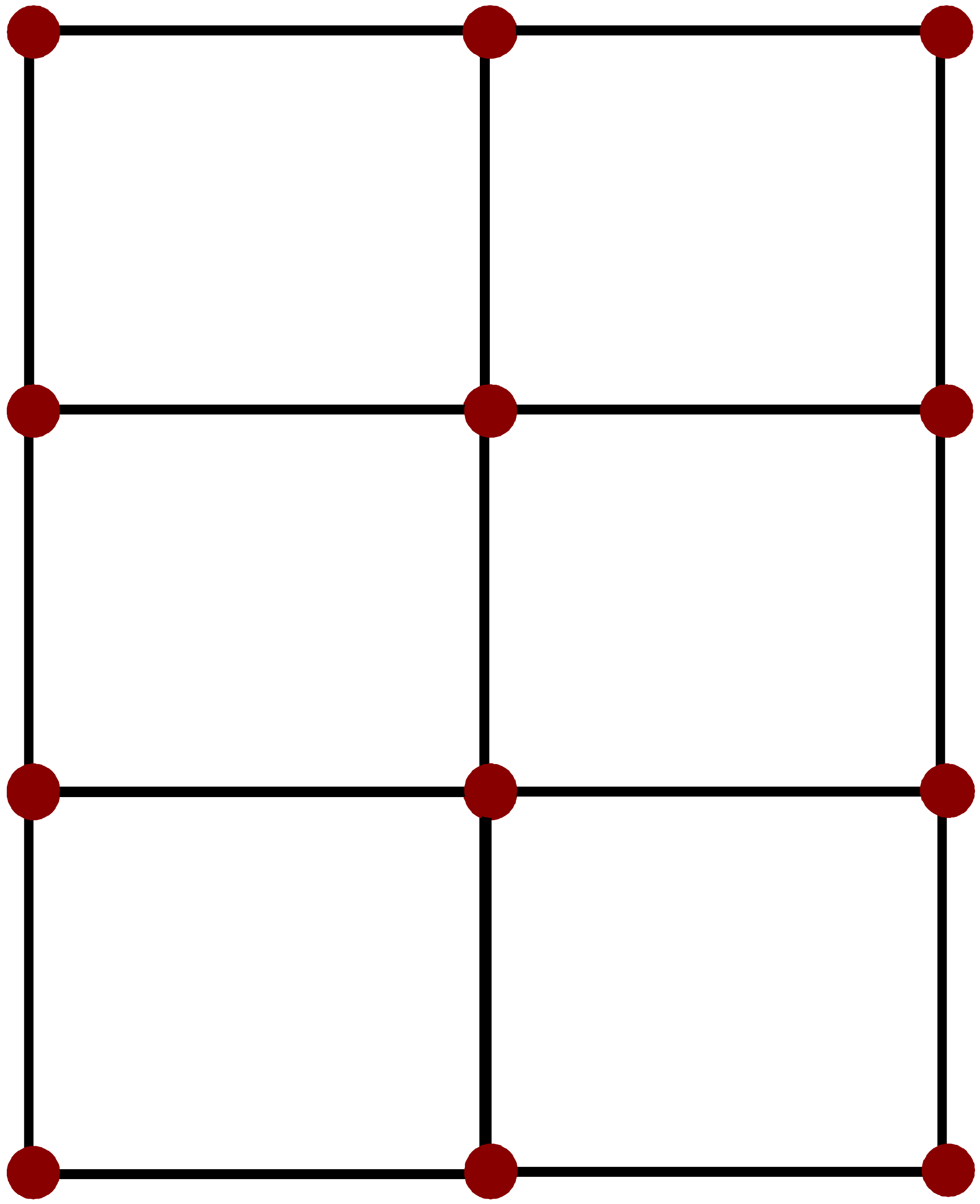
**Weak Form**

$$\int_{\Omega} q \nabla \cdot \boldsymbol{u} \, \mathrm{d}\Omega + T_{pspg} = 0$$

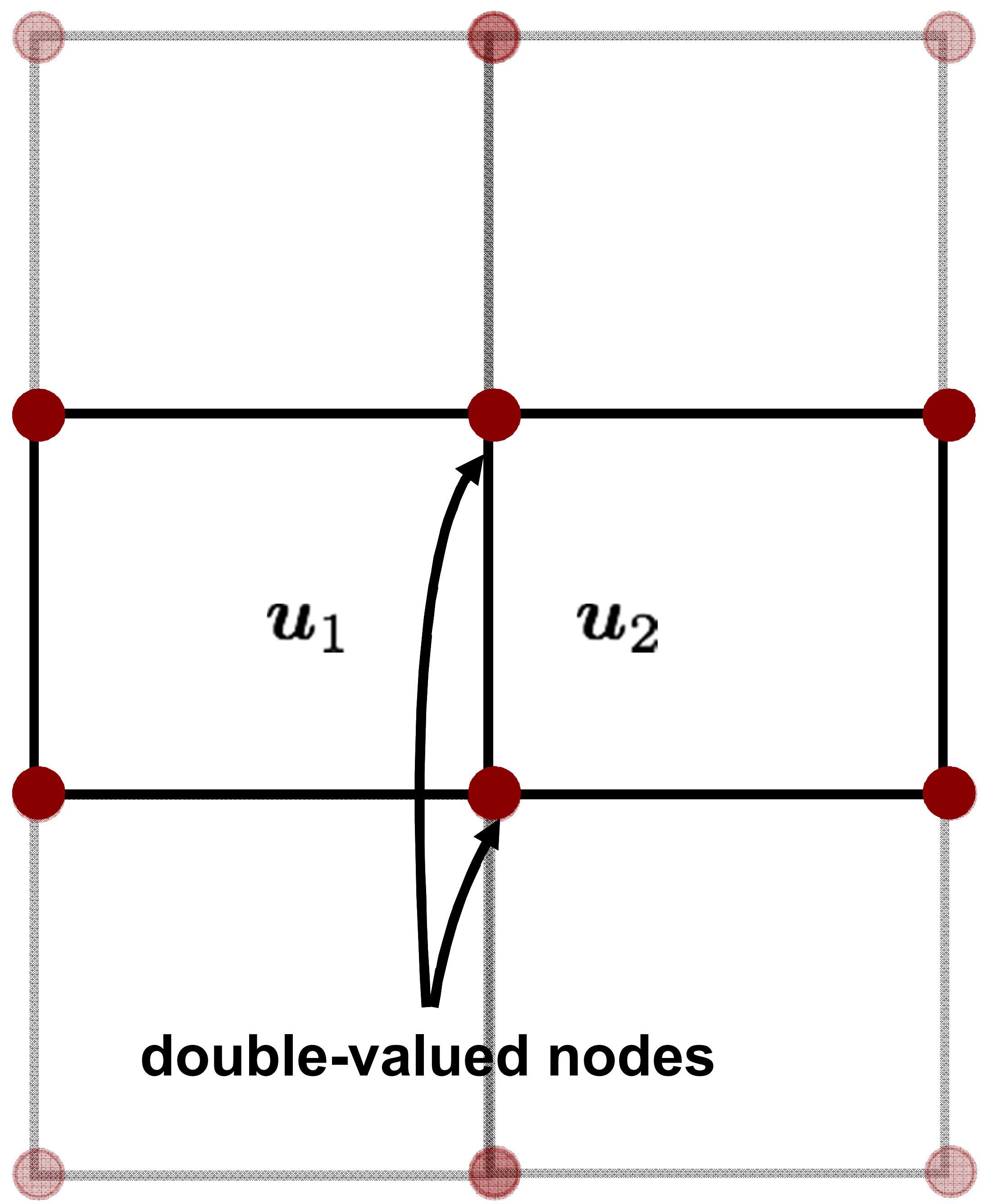
$$\int_{\Omega} \boldsymbol{w} \cdot \left( \rho \frac{\partial \boldsymbol{u}}{\partial t} + \rho \boldsymbol{u} \cdot \nabla \boldsymbol{u} - \boldsymbol{S} \right) \mathrm{d}\Omega$$

$$+ \int_{\Omega} \nabla \boldsymbol{w} : \boldsymbol{\sigma} \, \mathrm{d}\Omega - \int_{\partial\Omega} \boldsymbol{w} \cdot \boldsymbol{\sigma} \cdot \boldsymbol{n} \, \mathrm{d}s + T_{supg} = 0$$

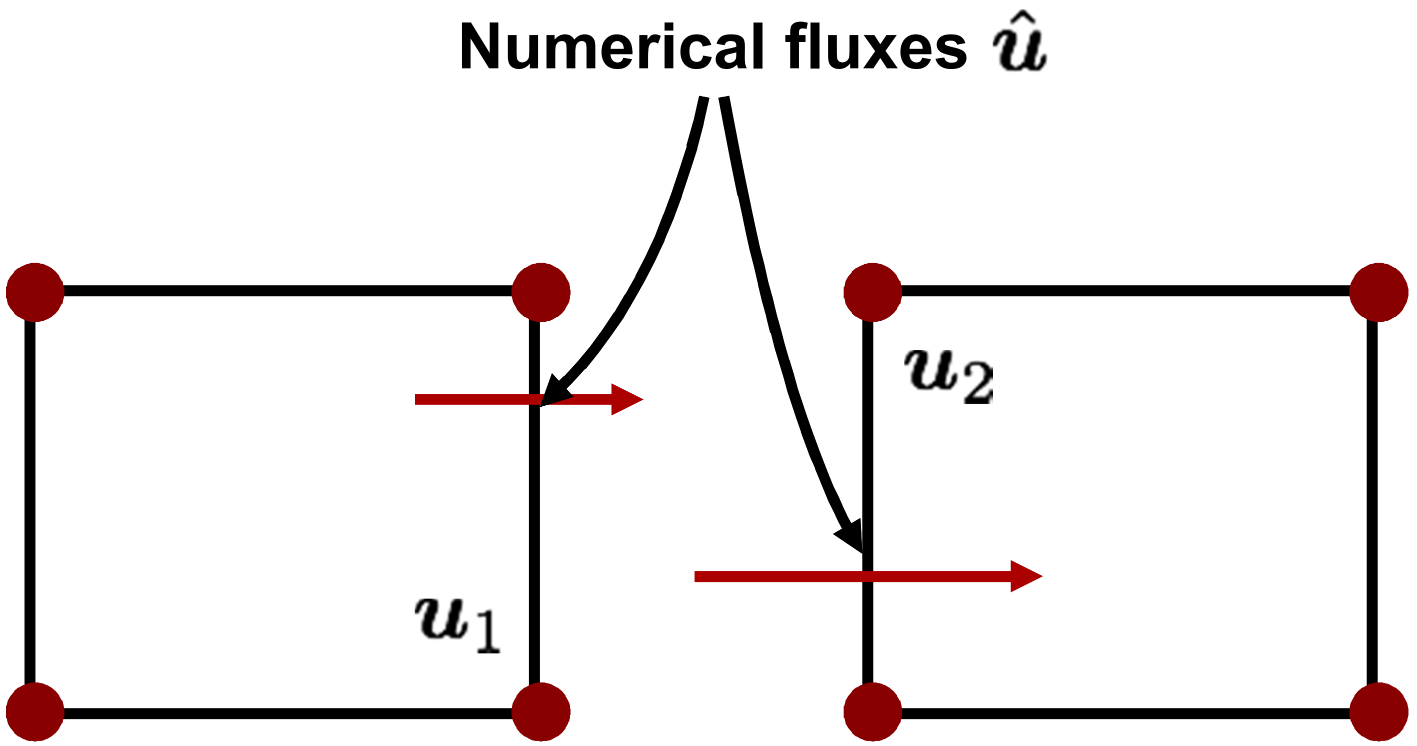
# DG-style Numerical Fluxes



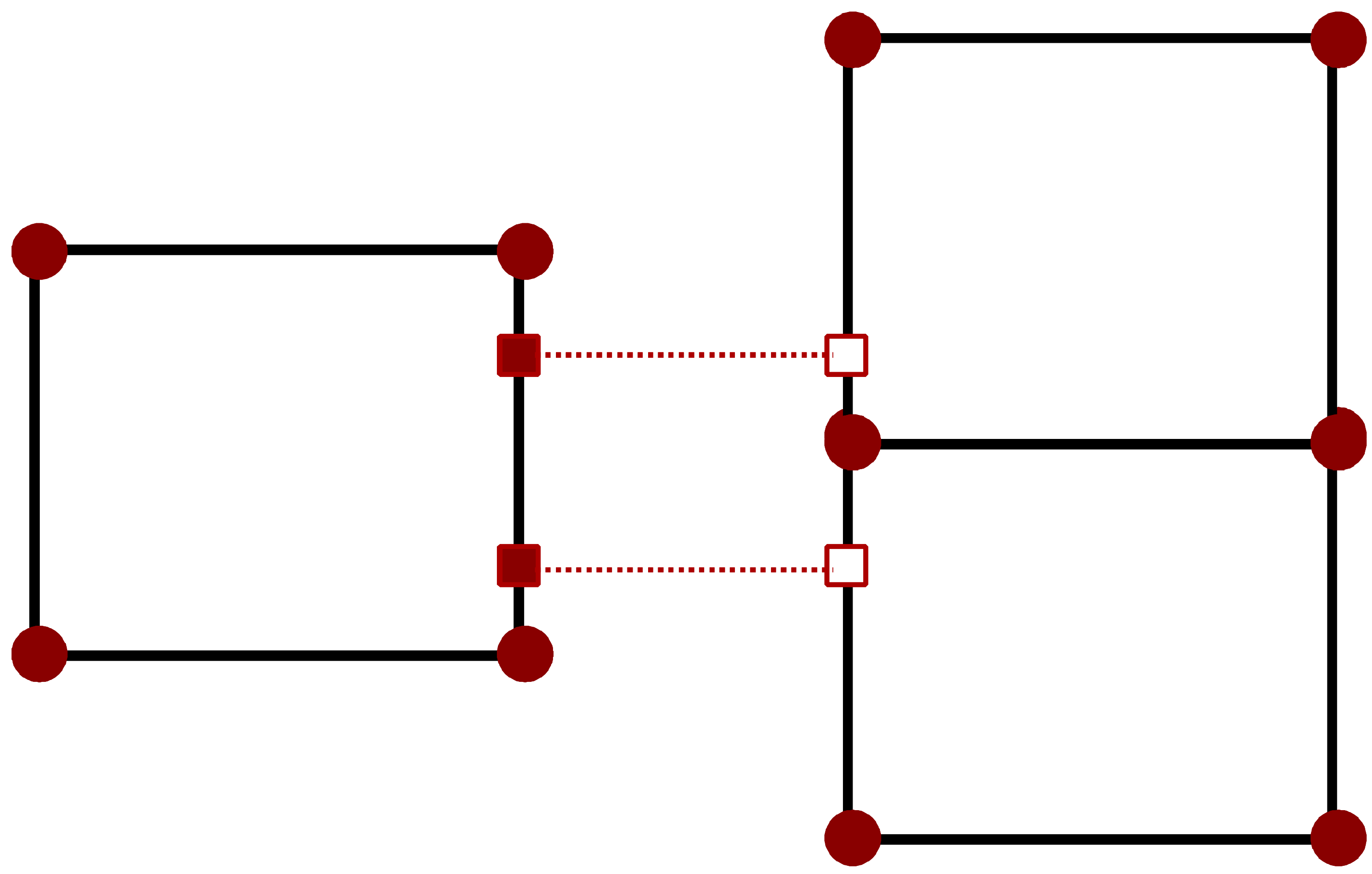
# DG-style Numerical Fluxes



# DG-style Numerical Fluxes



# DG-style Numerical Fluxes



# Continuity

not strictly conservative

$$\int_\Omega q \nabla \cdot \boldsymbol{u} \, \mathrm{d}\Omega + \dots$$

Integrate by parts with numerical flux

$$-\int_\Omega \nabla q \cdot \boldsymbol{u} \, \mathrm{d}\Omega + \sum_{K \in \mathcal{T}_h} \int_{\partial K} q_K \hat{\boldsymbol{u}}_K \cdot \boldsymbol{n}_K \, \mathrm{d}s + \dots$$

re-integrate with actual flux

$$\int_\Omega q \nabla \cdot \boldsymbol{u} \, \mathrm{d}\Omega + \sum_{K \in \mathcal{T}_h} \int_{\partial K} q_K \left( \hat{\boldsymbol{u}}_K - \boldsymbol{u}_K \right) \cdot \boldsymbol{n}_K \, \mathrm{d}s + \dots$$

# Continuity

not strictly conservative

$$\int_\Omega q \nabla \cdot \boldsymbol{u} \, \mathrm{d}\Omega + \ldots$$

$$\hat{\boldsymbol{u}} = \{\boldsymbol{u}\} + \lambda_c [\![P]\!]$$

Integrate by parts with numerical flux

$$-\int_\Omega \nabla q \cdot \boldsymbol{u} \, \mathrm{d}\Omega + \sum_{K \in \mathcal{T}_h} \int_{\partial K} q_K \hat{\boldsymbol{u}}_K \cdot \boldsymbol{n}_K \, \mathrm{d}s + \ldots$$

re-integrate with actual flux

$$\int_\Omega q \nabla \cdot \boldsymbol{u} \, \mathrm{d}\Omega + \sum_{K \in \mathcal{T}_h} \int_{\partial K} q_K \left( \hat{\boldsymbol{u}}_K - \boldsymbol{u}_K \right) \cdot \boldsymbol{n}_K \, \mathrm{d}s + \ldots$$

# Momentum Equation

$$\int_\Omega \boldsymbol{w} \cdot \left( \rho \frac{\partial \boldsymbol{u}}{\partial t} + \rho \boldsymbol{u} \cdot \nabla \boldsymbol{u} - \boldsymbol{S} \right) \mathrm{d}\Omega + \int_\Omega \nabla \boldsymbol{w} : \boldsymbol{\sigma} \, \mathrm{d}\Omega - \int_{\partial\Omega} \boldsymbol{w} \cdot \boldsymbol{\sigma} \cdot \boldsymbol{n} \, \mathrm{d}s + T_{supg} = 0$$

$$\int_\Omega \boldsymbol{w} \cdot \left( \rho \frac{\partial \boldsymbol{u}}{\partial t} + \rho \boldsymbol{u} \cdot \nabla \boldsymbol{u} - \boldsymbol{S} \right) \mathrm{d}\Omega + \int_\Omega \nabla \boldsymbol{w} : \boldsymbol{\sigma} \, \mathrm{d}\Omega - \sum_{K \in \mathcal{T}} \int_{\partial K} \boldsymbol{w}_K \cdot \hat{\boldsymbol{\sigma}}_K \cdot \boldsymbol{n}_K \, \mathrm{d}s + T_{supg} + \ldots = 0$$

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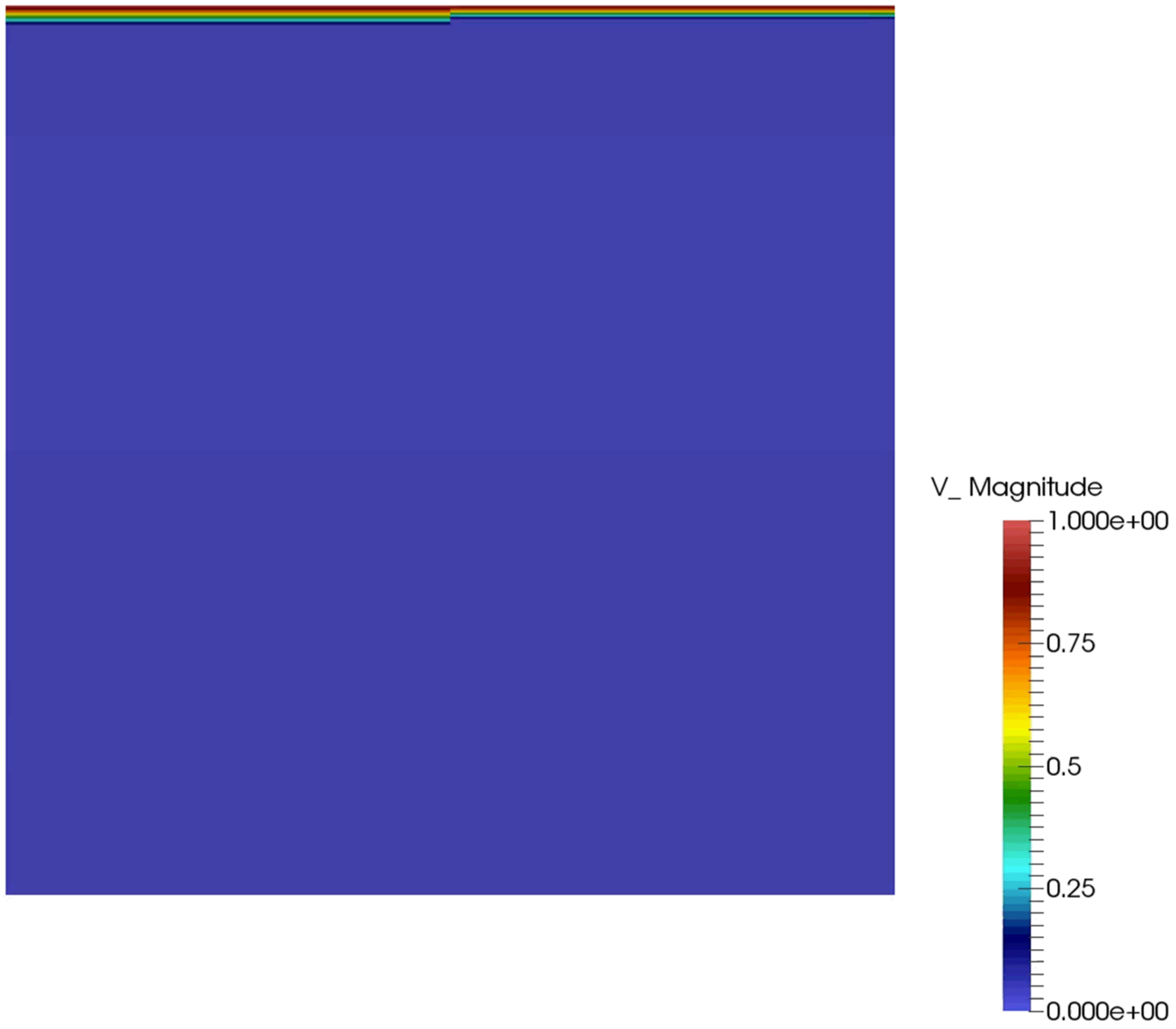
$$\int_\Omega \boldsymbol{w} \cdot \left( \rho \frac{\partial \boldsymbol{u}}{\partial t} + \rho \boldsymbol{u} \cdot \nabla \boldsymbol{u} - \boldsymbol{S} \right) \mathrm{d}\Omega + \int_\Omega \nabla \boldsymbol{w} : \boldsymbol{\sigma} \, \mathrm{d}\Omega - \int_{\partial\Omega} \boldsymbol{w} \cdot \boldsymbol{\sigma} \cdot \boldsymbol{n} \, \mathrm{d}s + T_{supg} = 0$$

$$\int_\Omega \boldsymbol{w} \cdot \left( \rho \frac{\partial \boldsymbol{u}}{\partial t} + \rho \boldsymbol{u} \cdot \nabla \boldsymbol{u} - \boldsymbol{S} \right) \mathrm{d}\Omega + \int_\Omega \nabla \boldsymbol{w} : \boldsymbol{\sigma} \, \mathrm{d}\Omega - \sum_{K \in \mathcal{T}} \int_{\partial K} \boldsymbol{w}_K \cdot \hat{\boldsymbol{\sigma}}_K \cdot \boldsymbol{n}_K \, \mathrm{d}s + T_{supg} + \ldots = 0$$

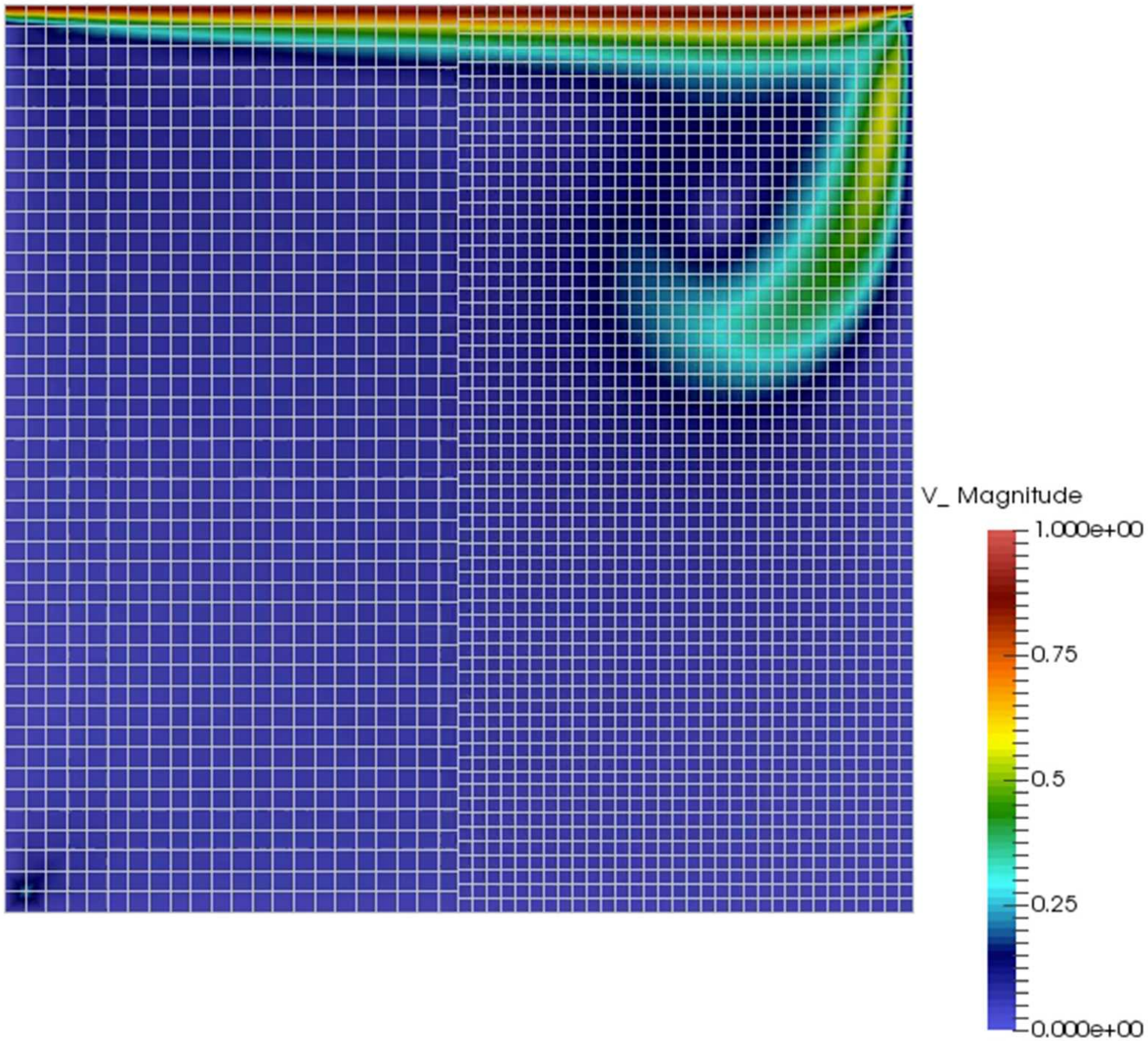
$$\boxed{\hat{\boldsymbol{\sigma}} = \{\boldsymbol{\sigma}\} + \lambda_m [\![\boldsymbol{u}]\!]}$$

Arnold et al. 2002 SIAM J. Numer. Anal., 39, 1749–79.
Domino, S.P. 2010 Center for Turbulence Research Summer Program.

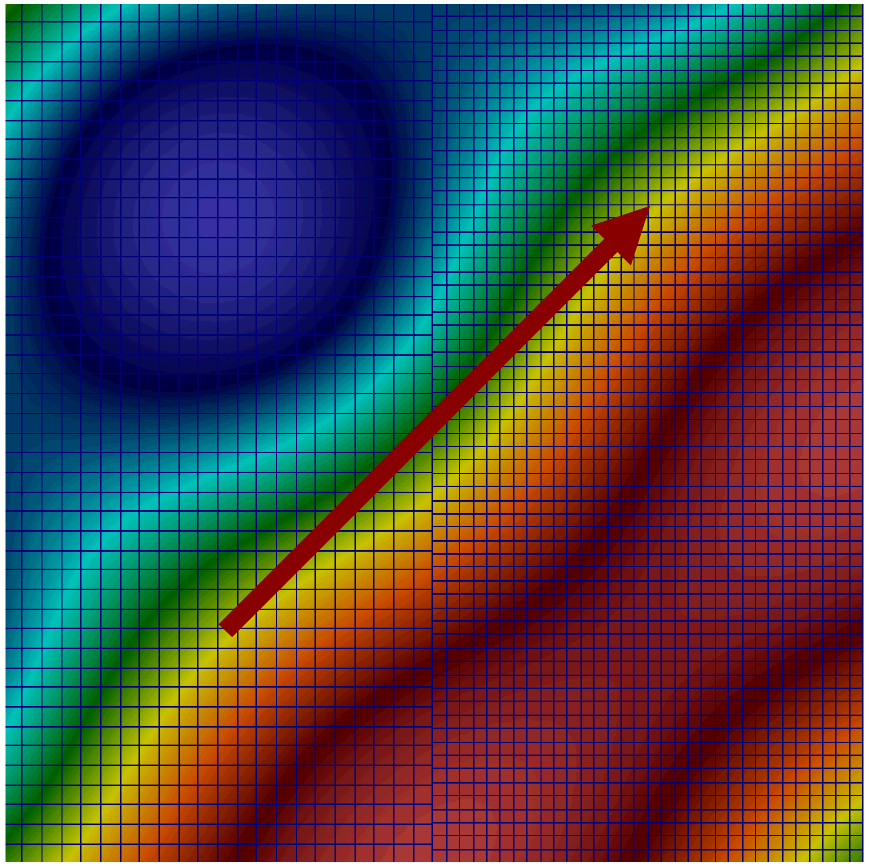
# Lid-driven Cavity Flow



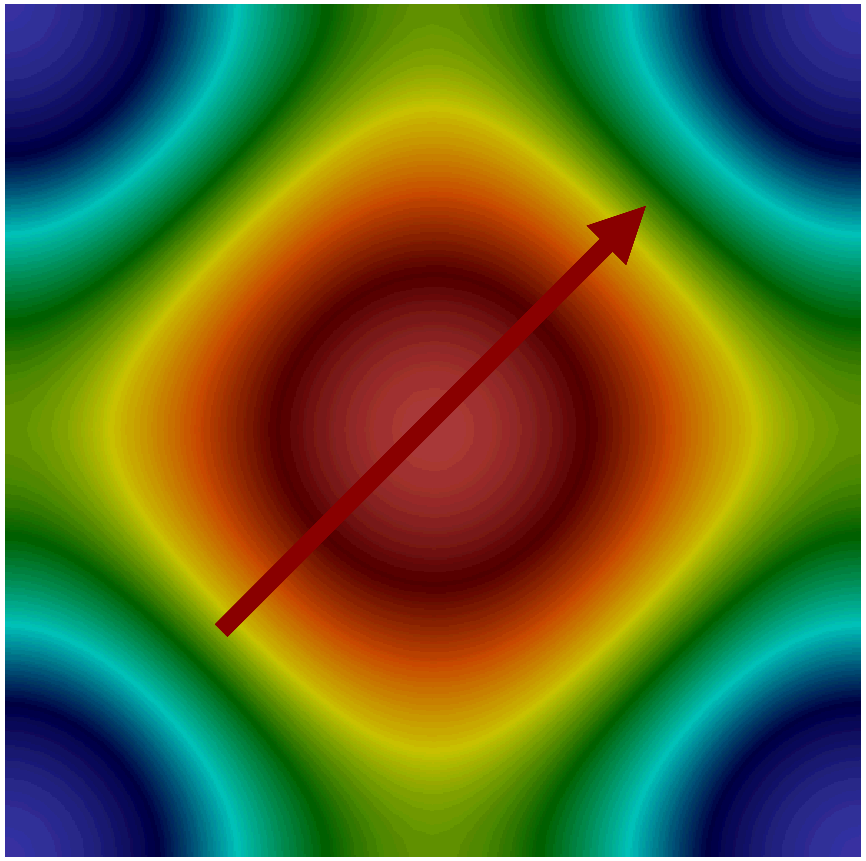
# Lid-driven Cavity Flow



# Convecting Taylor Vortex



velocity

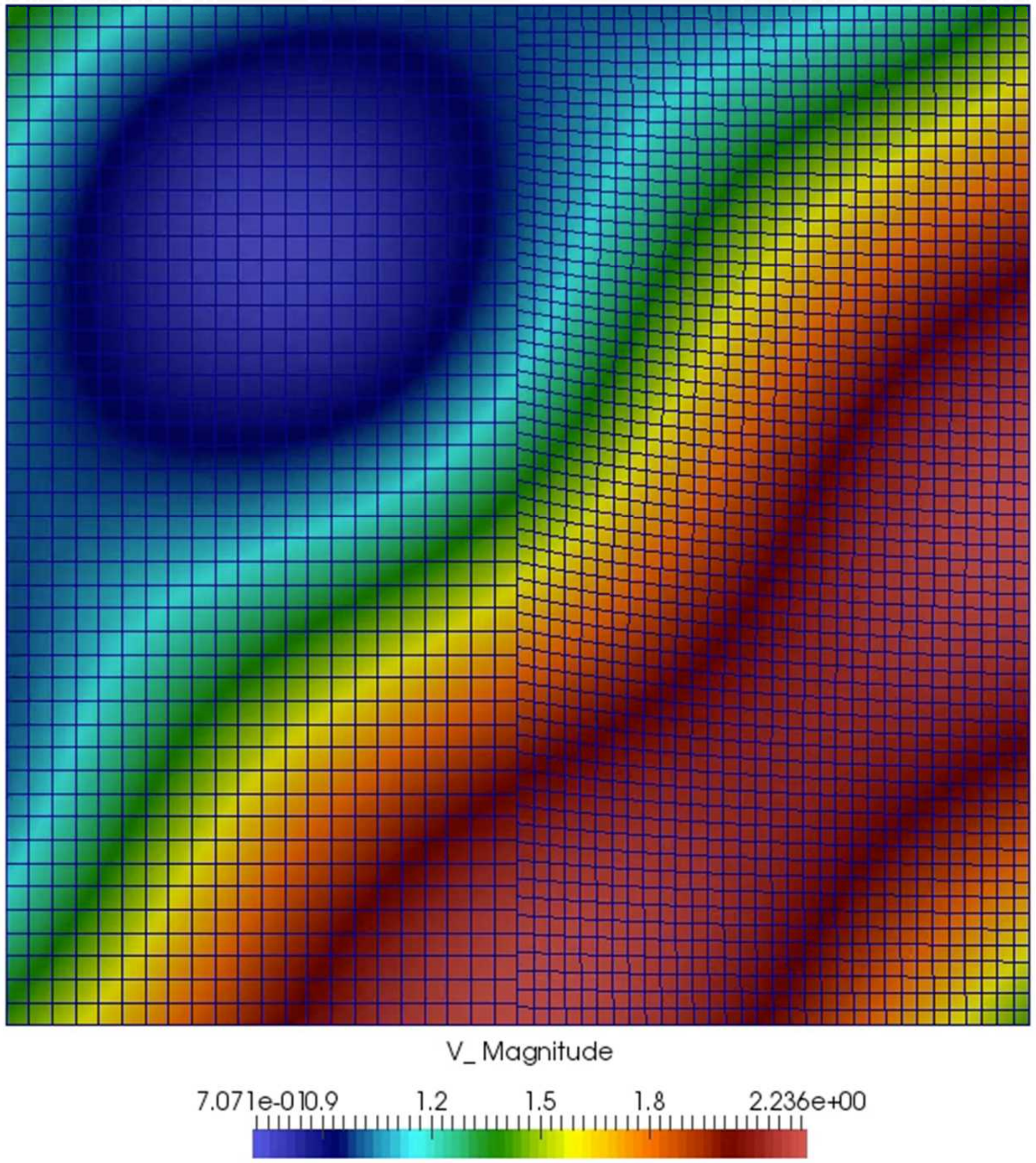


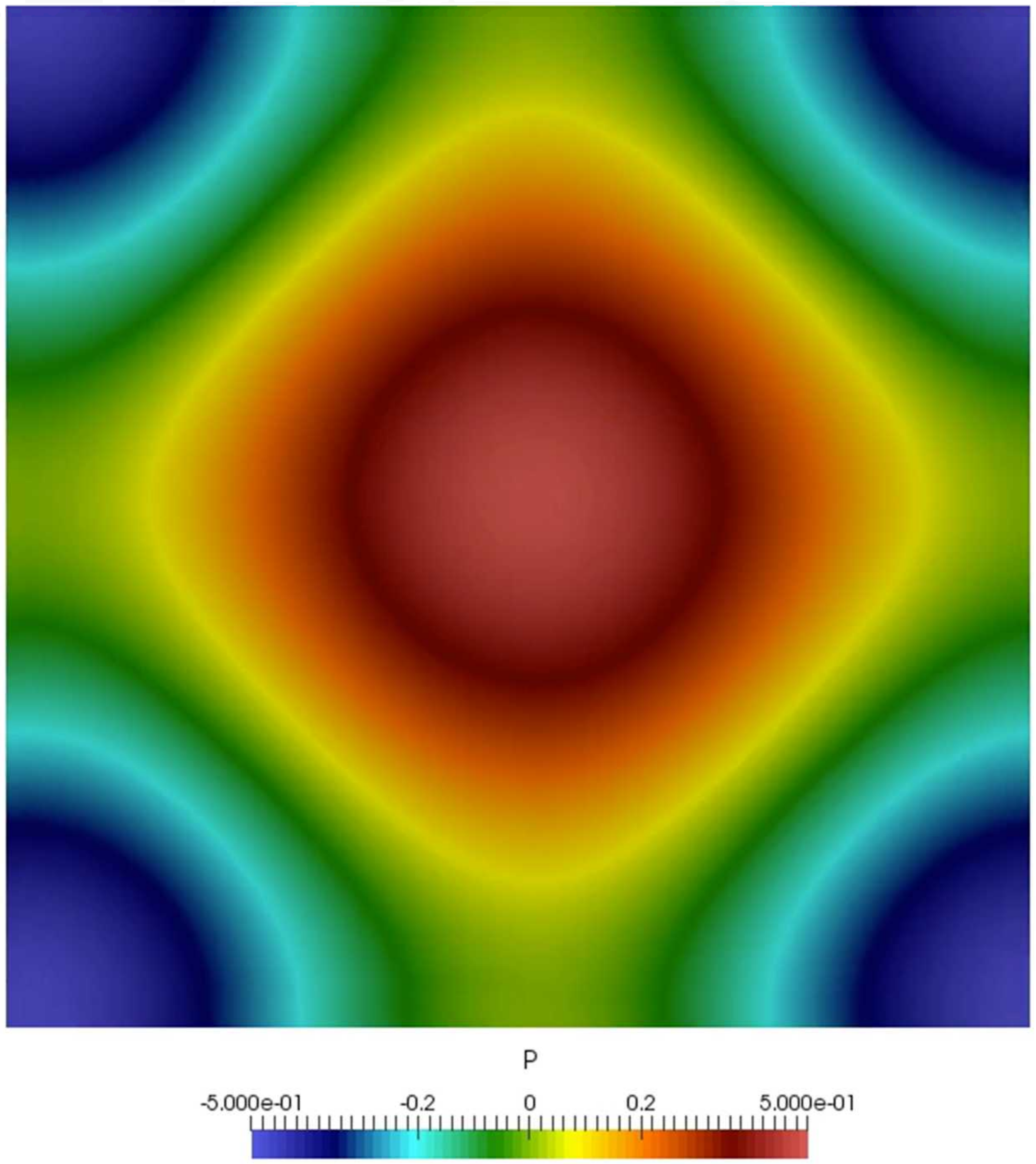
pressure

$$u = 1 - \cos\left[\pi\left(x-t\right)\right]\sin\left[\pi\left(y-t\right)\right]\exp\left(-2\pi^2/\mathrm{Re}\right)$$
$$v = 1 + \sin\left[\pi\left(x-t\right)\right]\cos\left[\pi\left(y-t\right)\right]\exp\left(-2\pi^2/\mathrm{Re}\right)$$
$$P = -\tfrac{1}{4}\left\{\cos\left[2\pi\left(x-t\right)\right]+\cos\left[2\pi\left(y-t\right)\right]\right\}\exp(-4\pi^2/\mathrm{Re})$$

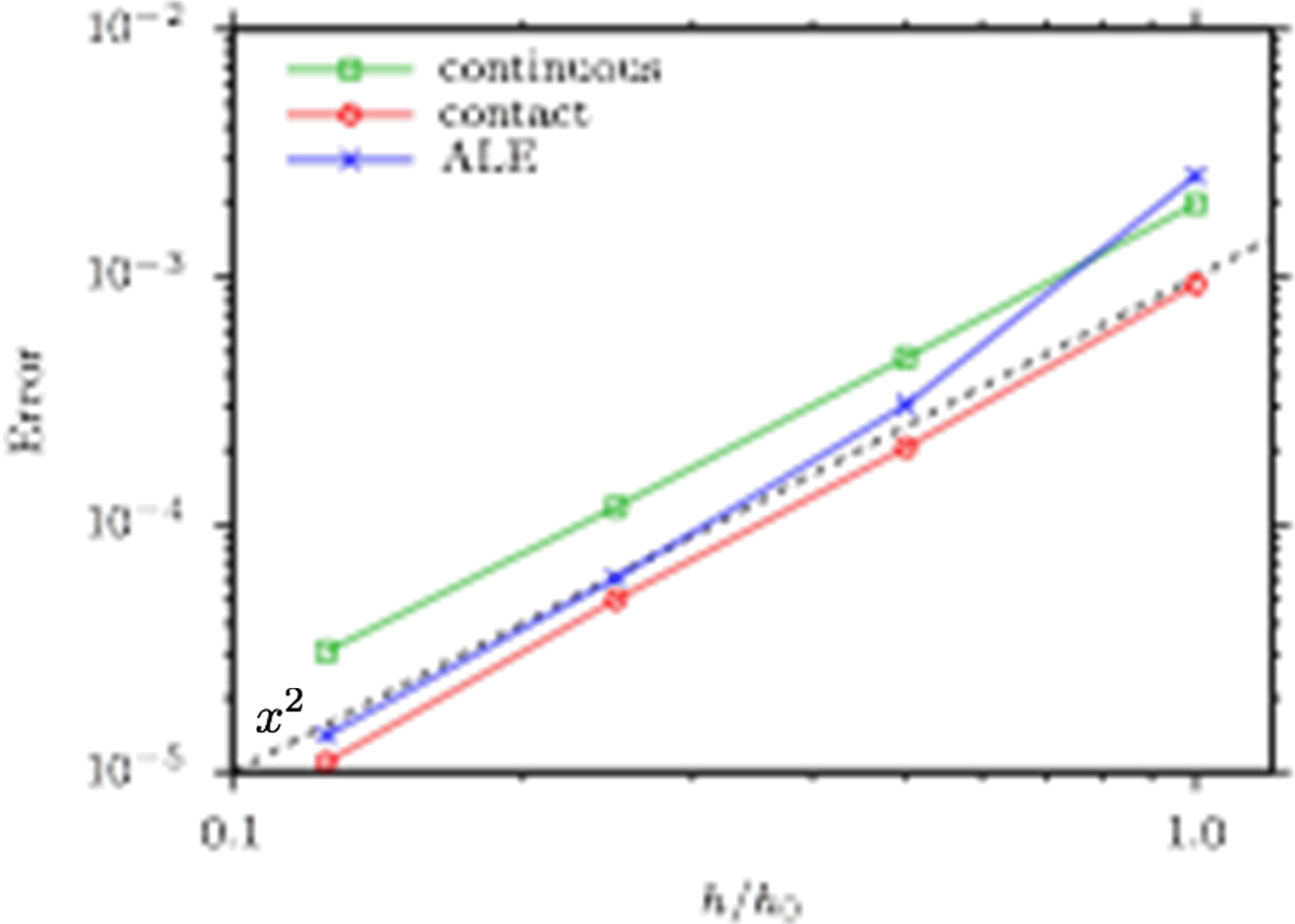
Re 1000
t = 1

# Convecting Taylor Vortex

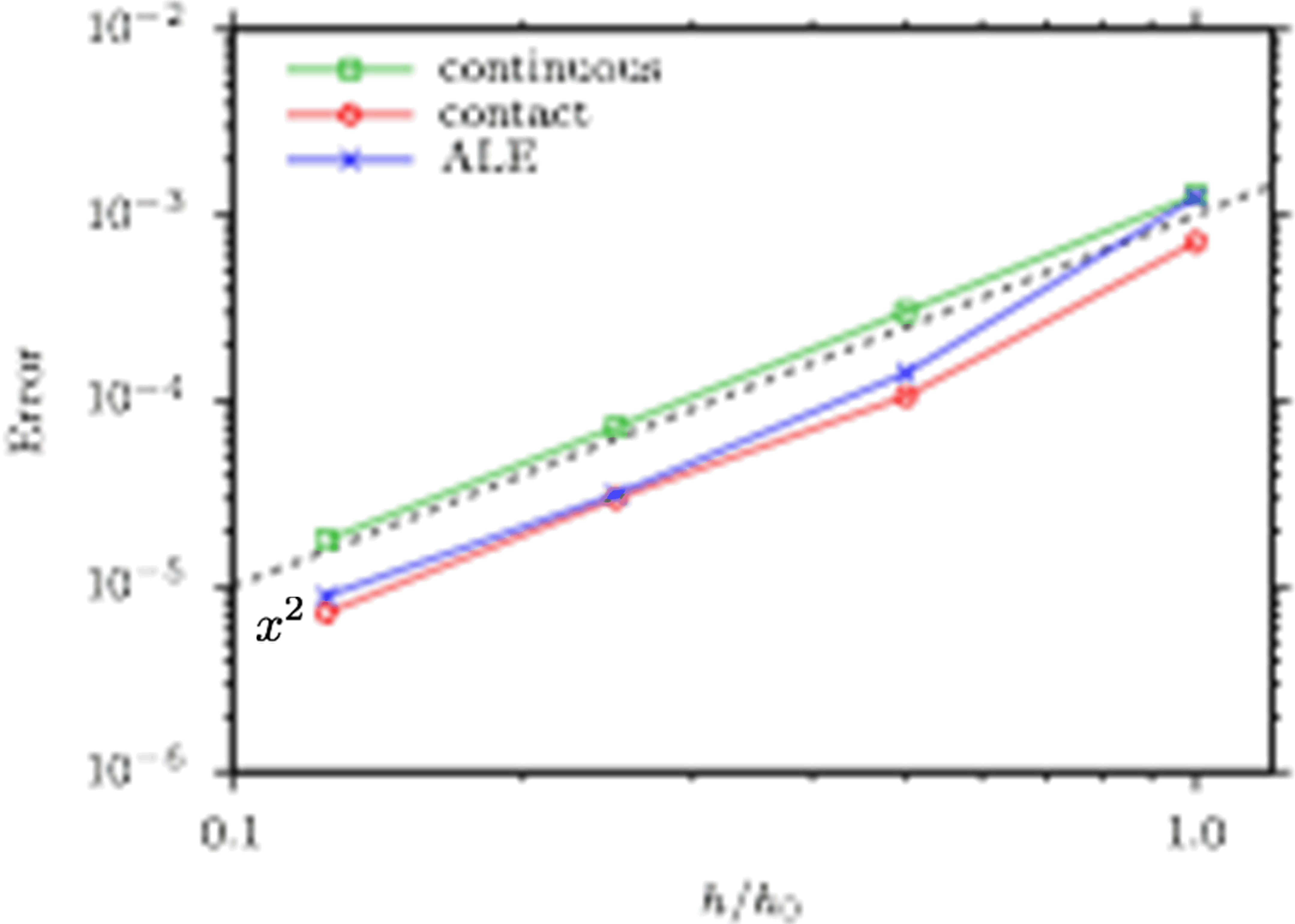


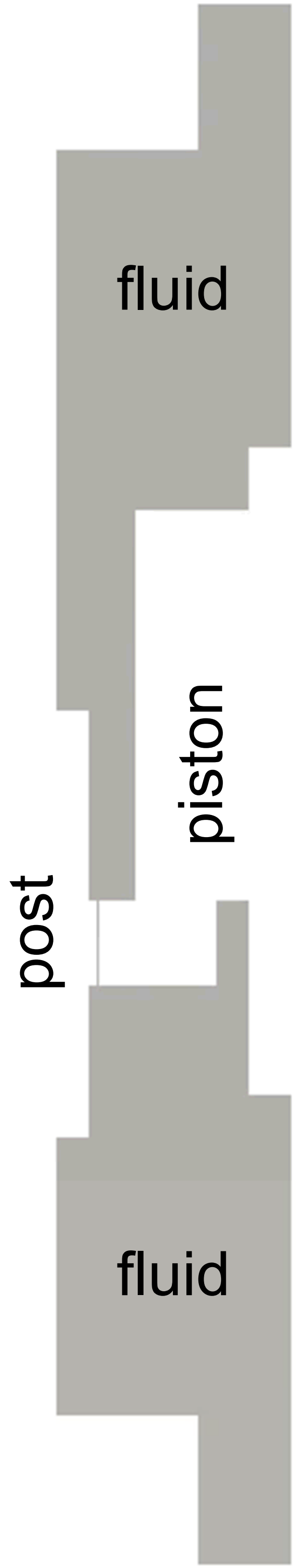
# Velocity Errors

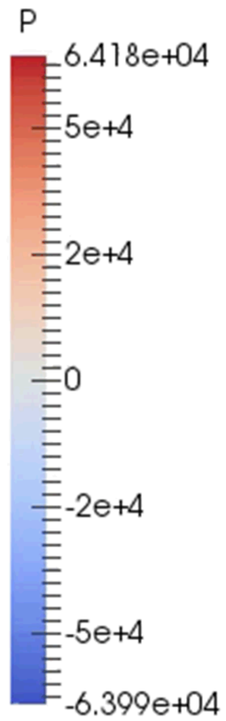


# Pressure Errors



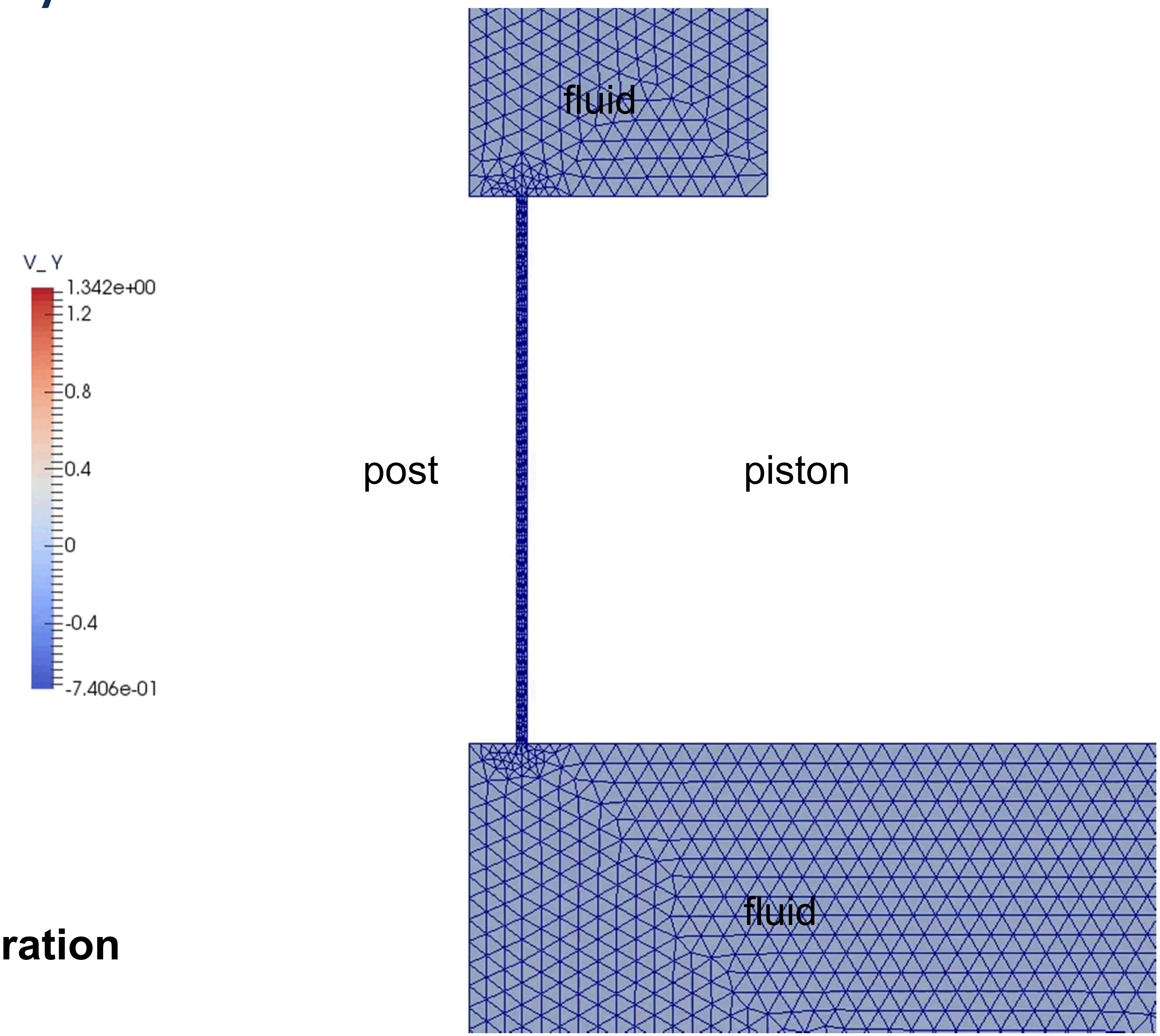
# Piston System




**10 g acceleration**
**100 Hz**

# Piston System




**10 g acceleration**
**100 Hz**

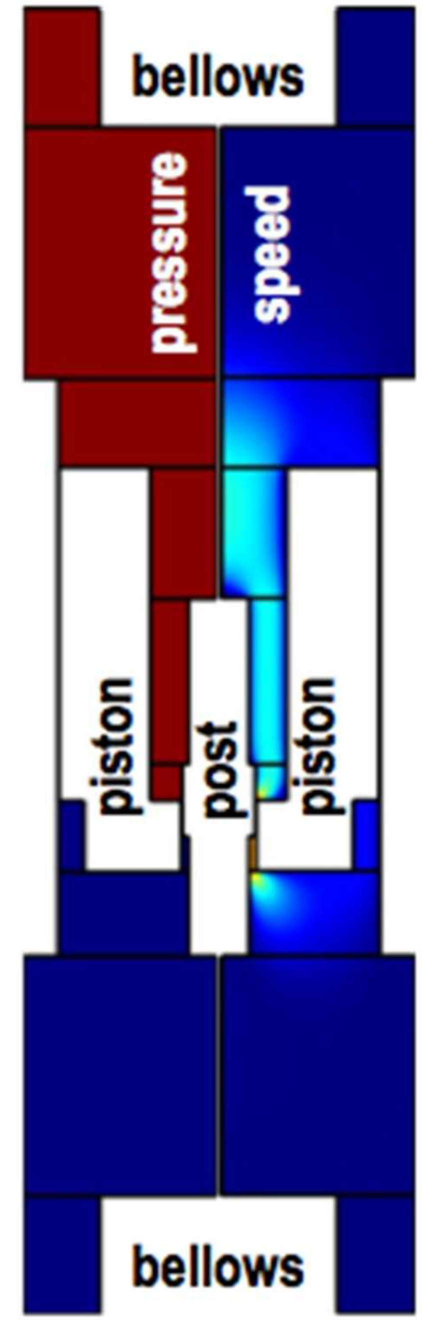
# Reduced-Order Model

$$\frac{d}{dt}\left((\bar{\mathbf{M}}+\mathbf{M})\frac{d\mathbf{Z}}{dt}\right)+\mathbf{B}\frac{d\mathbf{Z}}{dt}+\bar{\mathbf{K}}\mathbf{Z}=\mathbf{F}\ ,\ \mathbf{Z}=\begin{pmatrix}Z_p\\ Z_s\end{pmatrix}$$

$$\bar{\mathbf{M}}=\begin{pmatrix}M_p & 0\\ 0 & M_s\end{pmatrix},\ \bar{\mathbf{K}}=\begin{pmatrix}K_p & 0\\ 0 & K_s\end{pmatrix}$$

$$\mathbf{M}=\left(M_{ij}\right),\ \mathbf{B}=\left(B_{ij}\right)$$

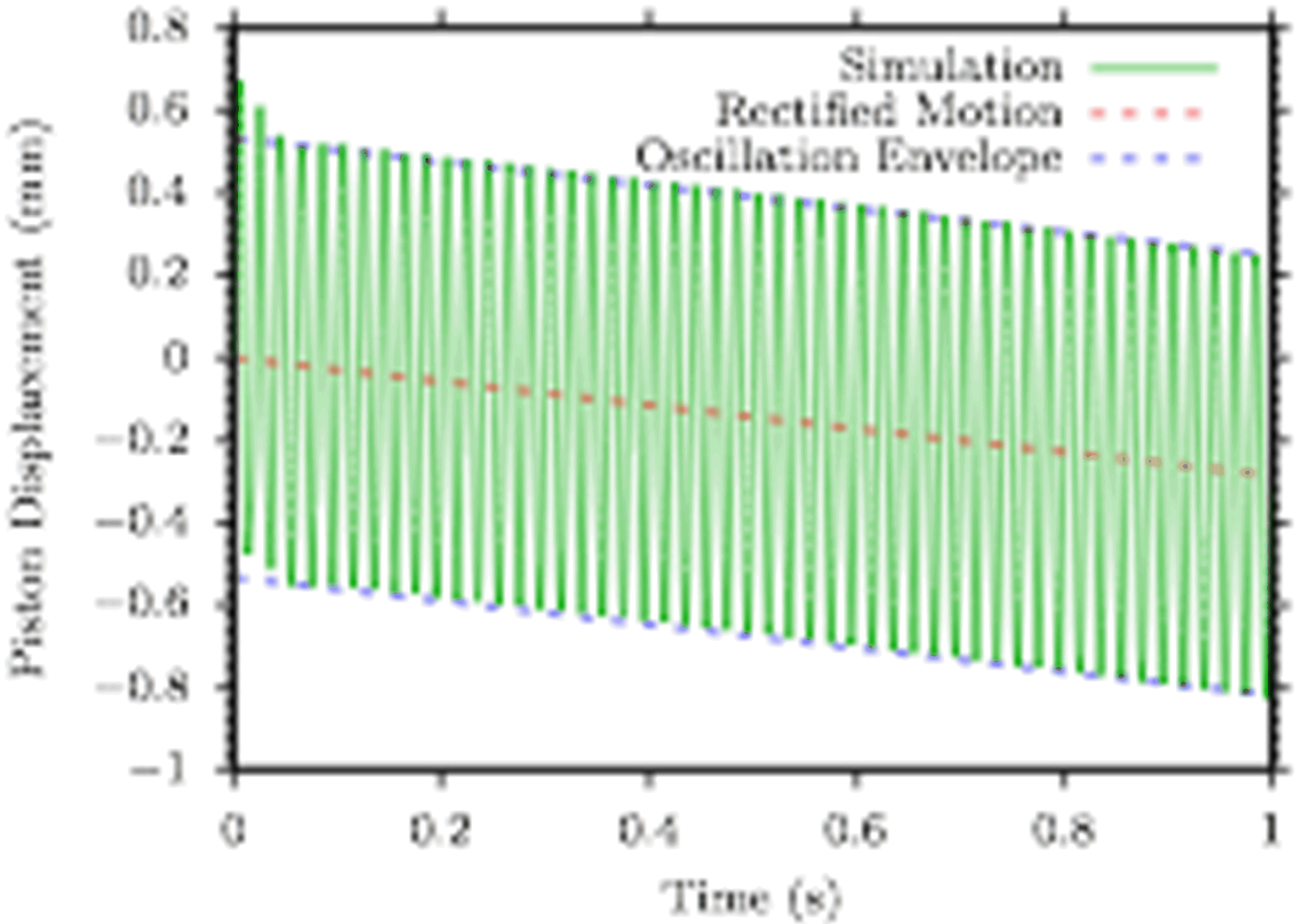
$$\mathbf{F}=-\begin{pmatrix}M_p-M_{LP}\\ M_{IP}+M_V\end{pmatrix}g_1\sin\left[\omega t\right]$$

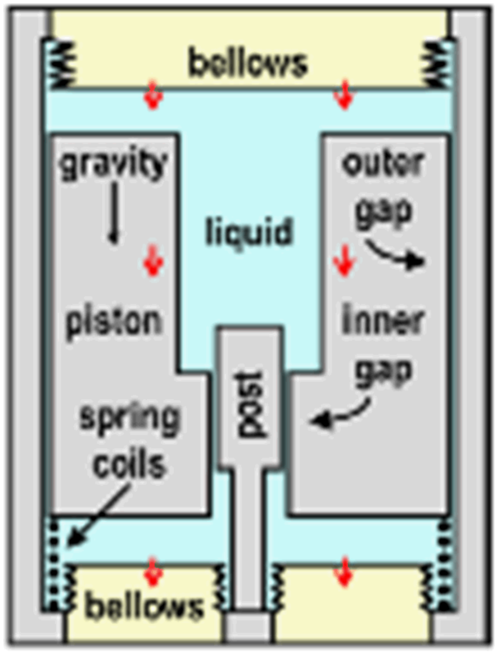



Romero et al. 2016 Gas-enabled resonance and rectified motion of a piston in a vibrated housing filled with a visc

# Comparison with ROM

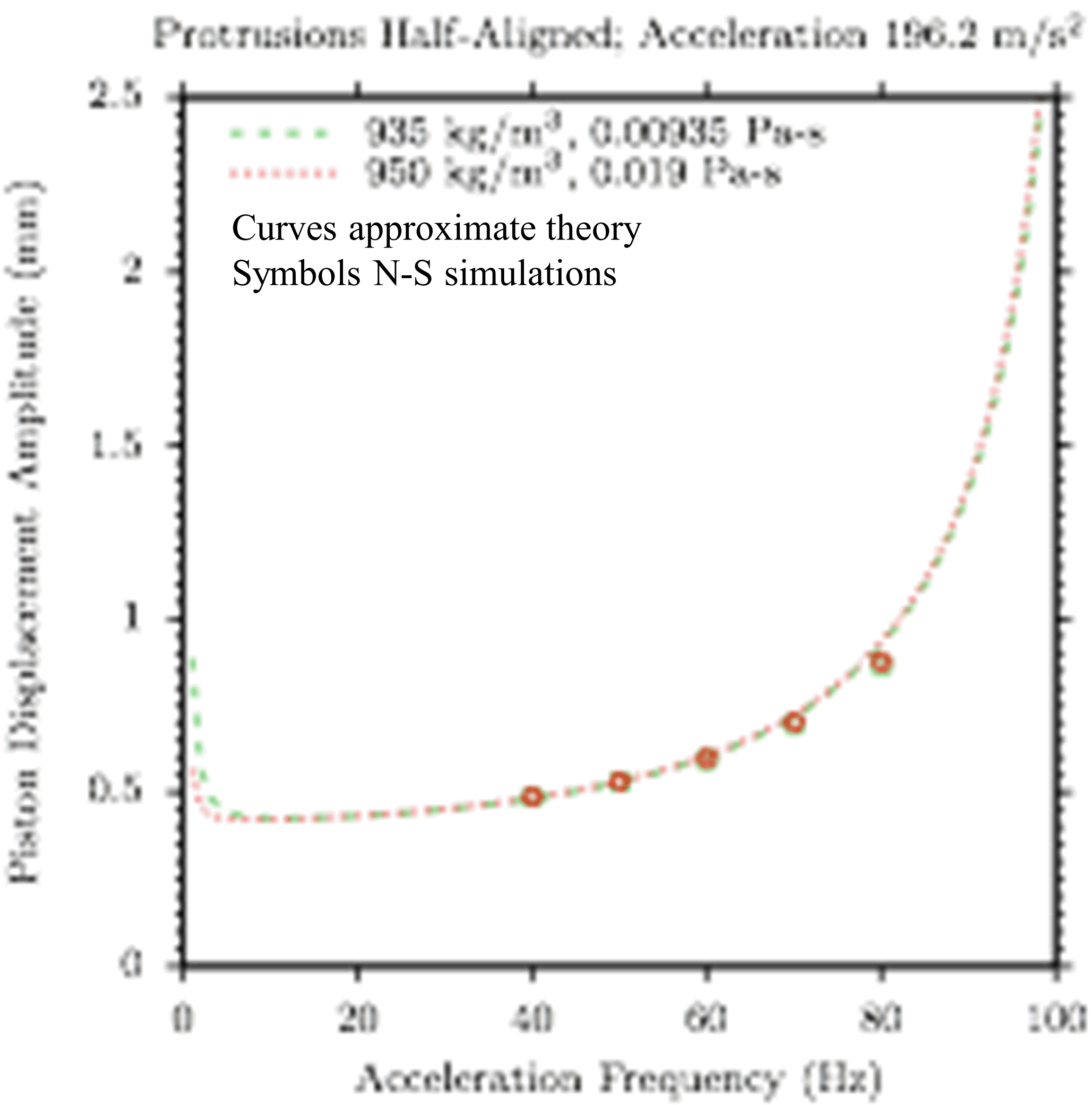
Protrusions Half-Aligned
196.2 m/s$^2$, 50 Hz, 950 kg/m$^3$, 0.019 Pa-s

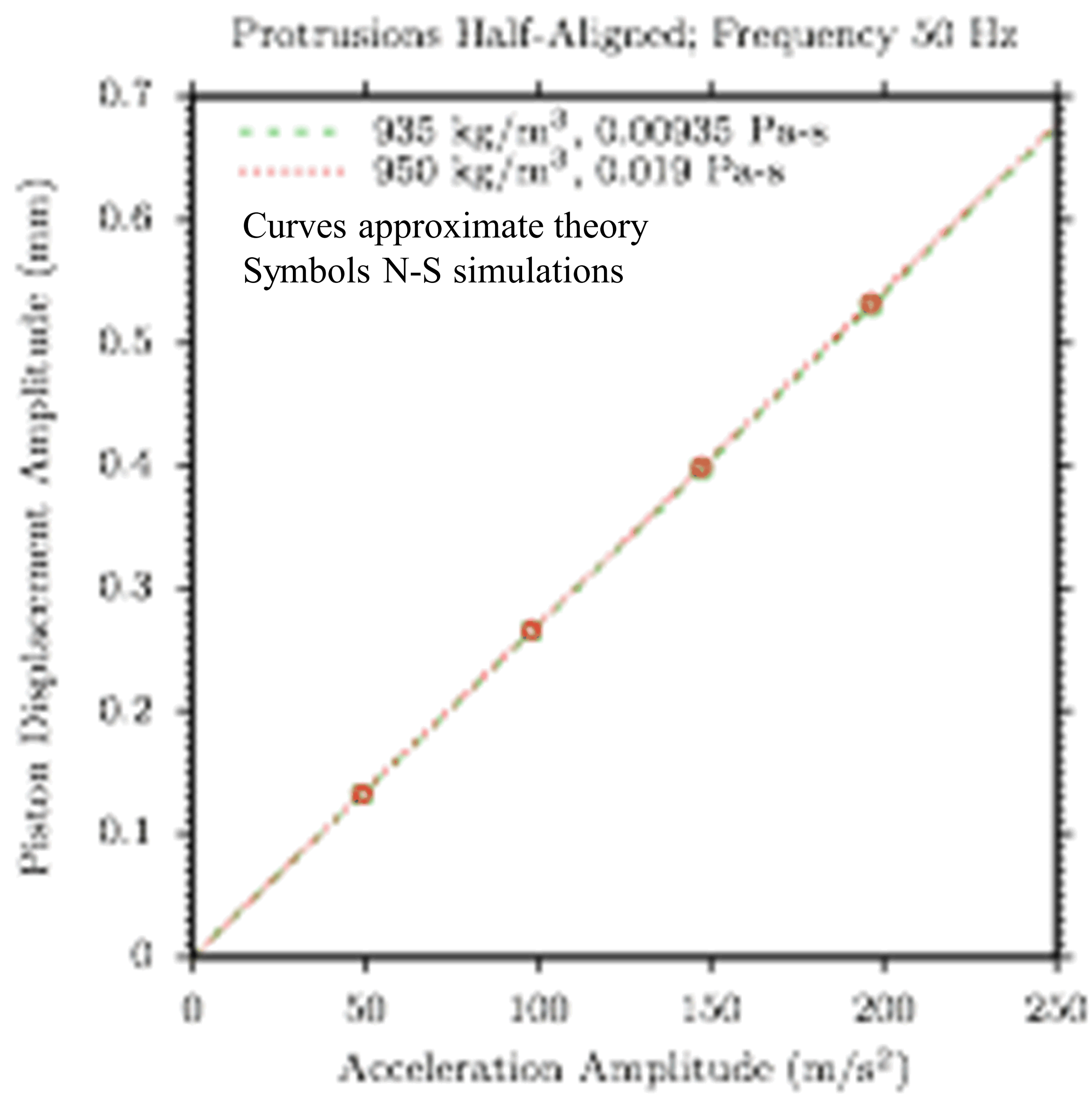


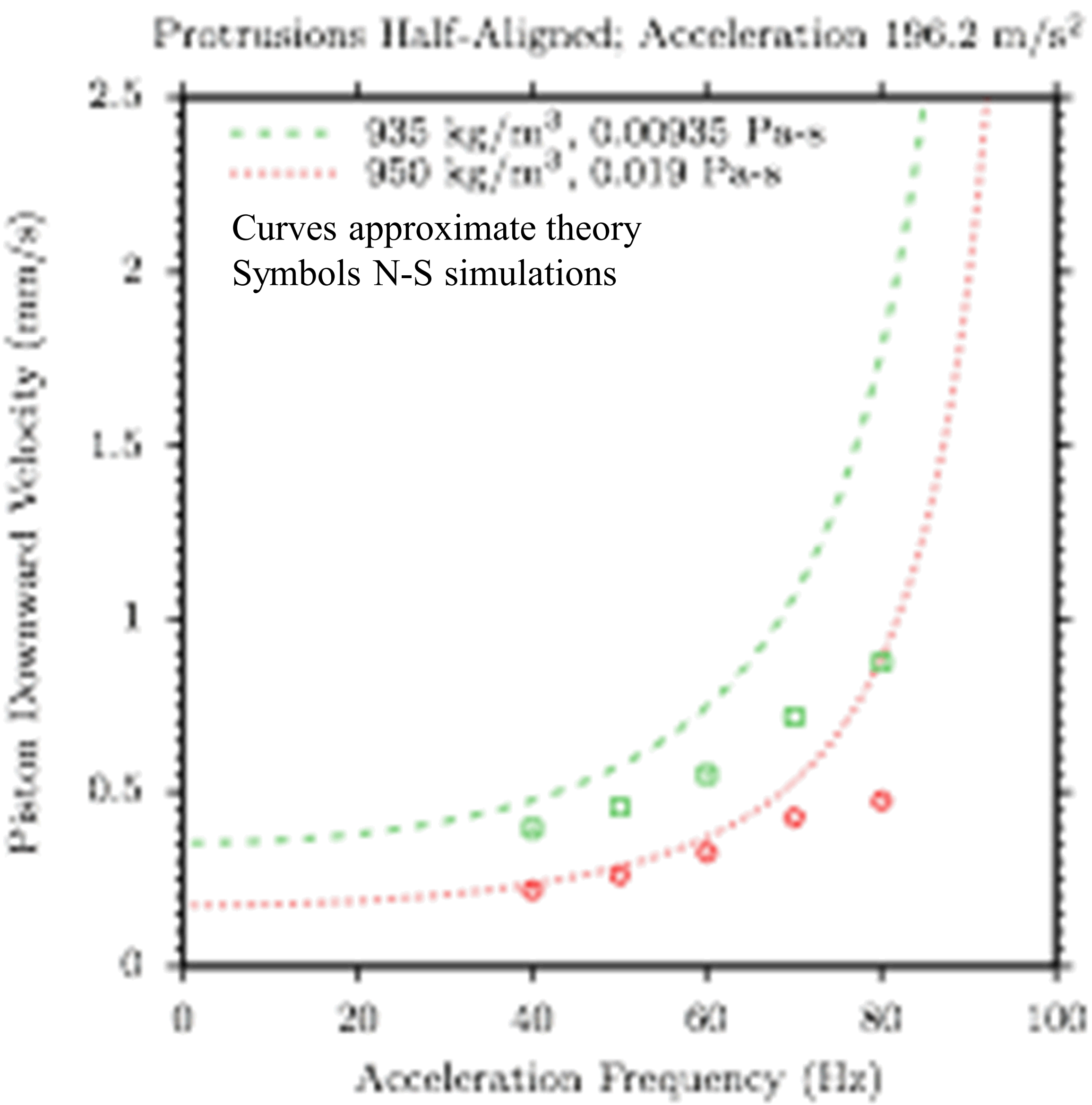

Romero et al. 2016 Gas-enabled resonance and rectified motion of a piston in a vibrated housing filled with a visc

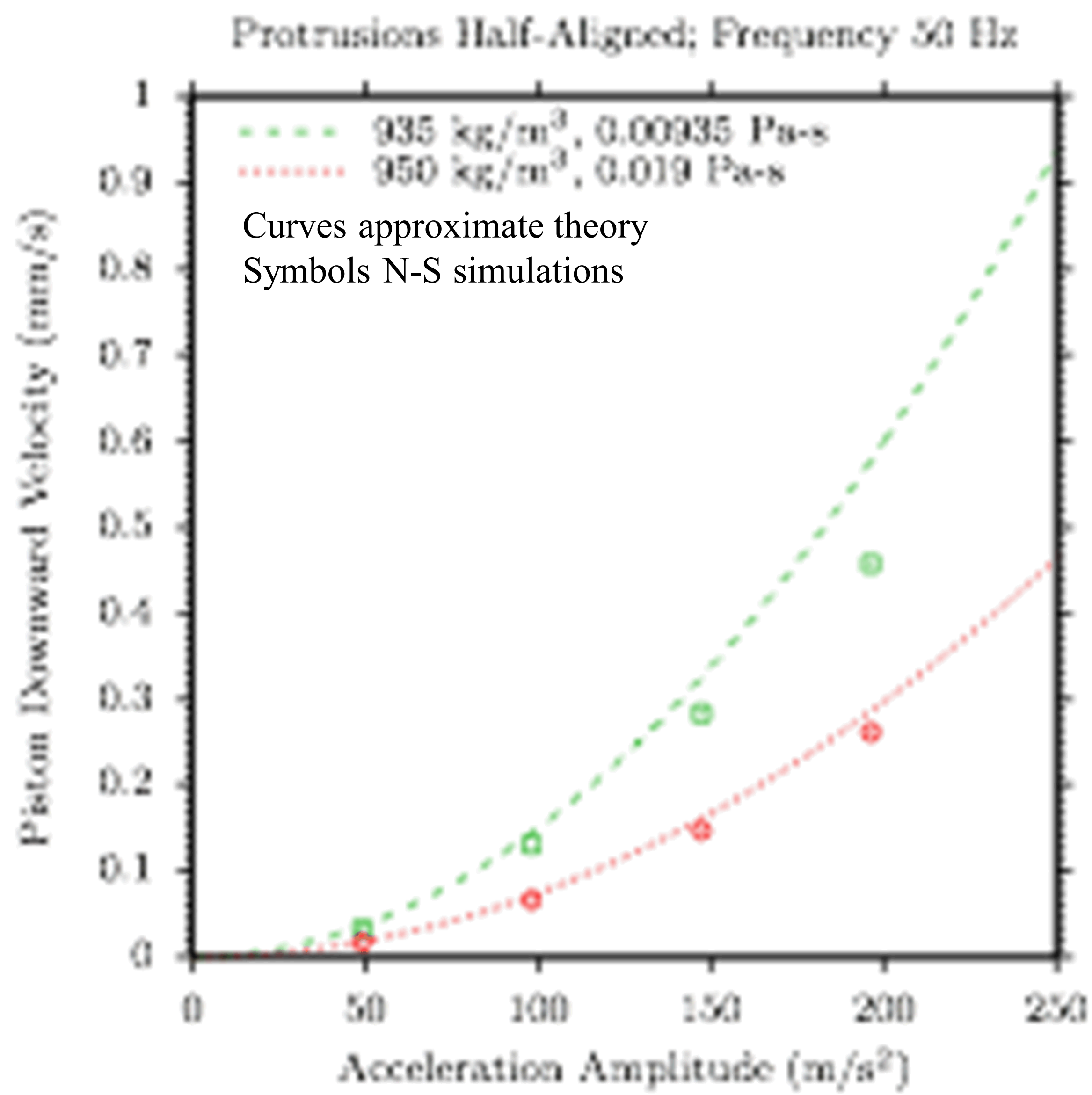
# Comparison with ROM



# Comparison with ROM



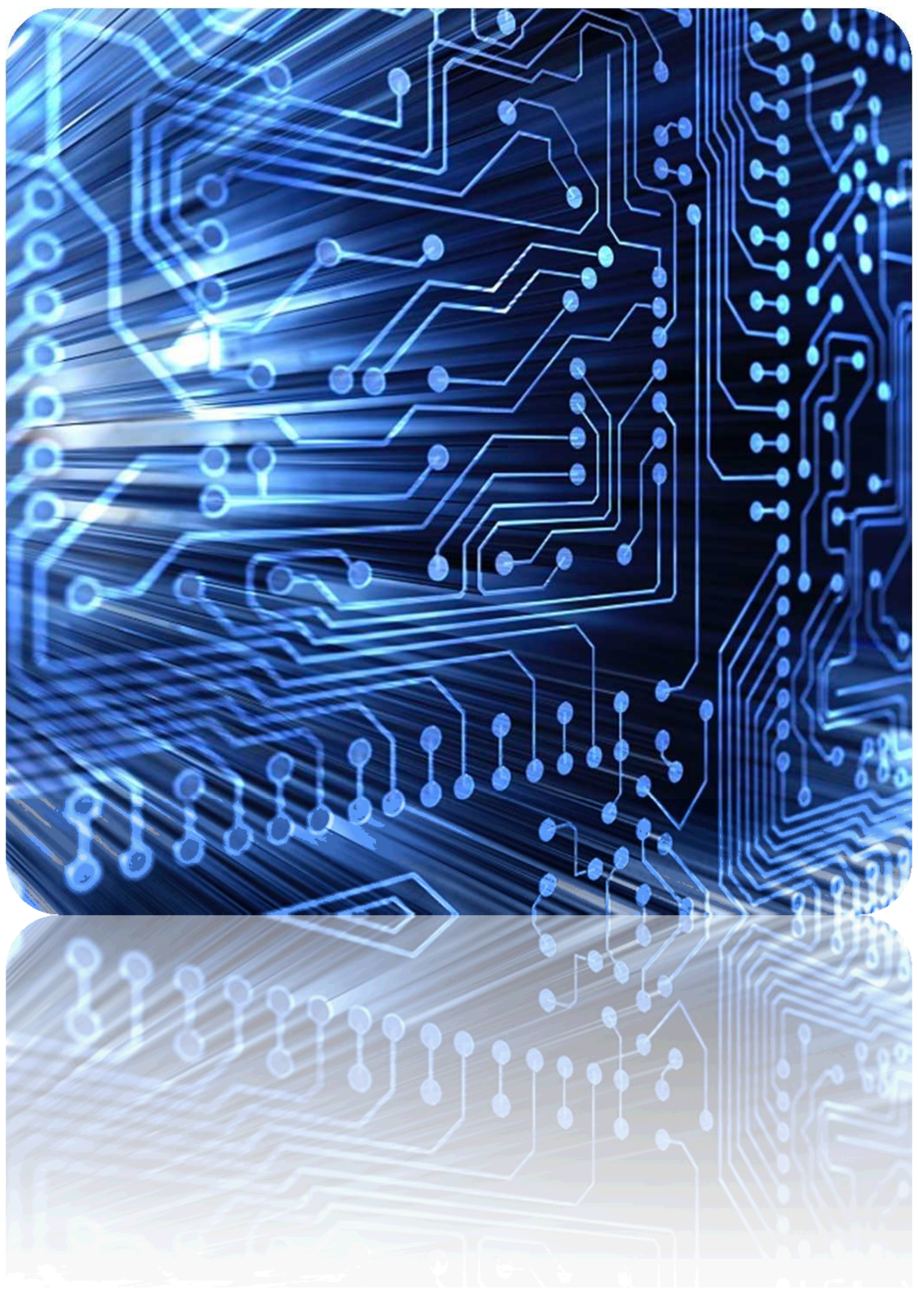
# Outline

- Sierra Mechanics
- Piston–fluid system
- **Next-generation platforms**

# Sandia's Codes



MPI



# How to transition to NGP



- portable/performance
- heterogeneous architectures
- MPI + X
- OpenMP
  - not proven on GPUs
  - does not handle memory hierarchies
- Kokkos

# Kokkos

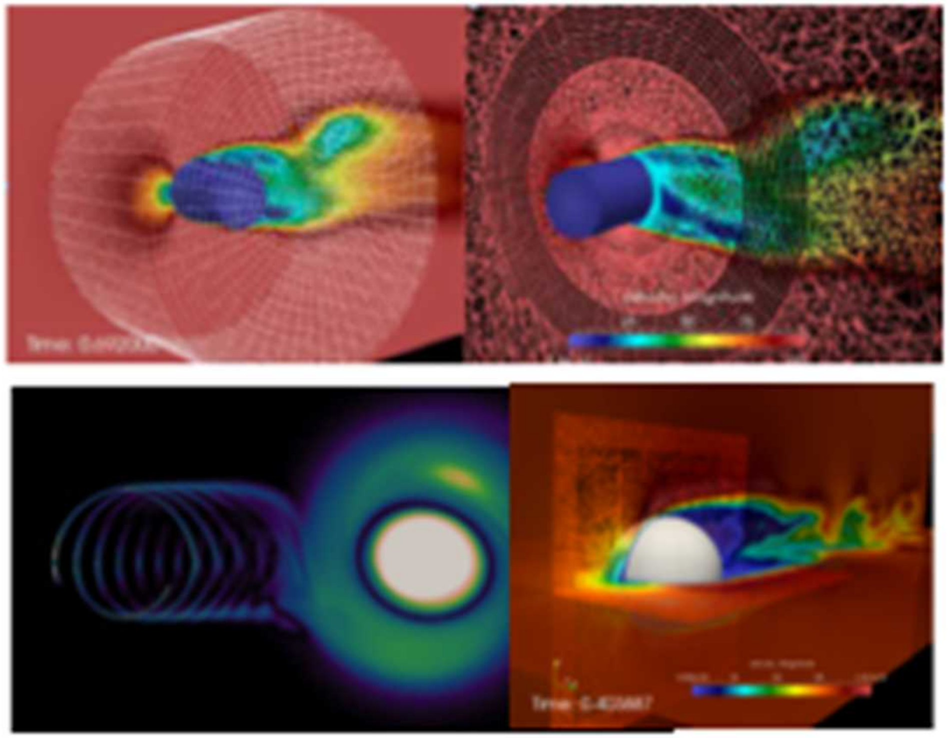
- Goal: performance portability
  - one code, multiple architectures
  - performant memory access patterns
  - architecture-specific features
- provides
  - parallel execution policy
  - architecture-aware data structures
- backends
  - OpenMP
  - Cuda
- open source
  - https://github.com/kokkos

Sandia National Laboratories

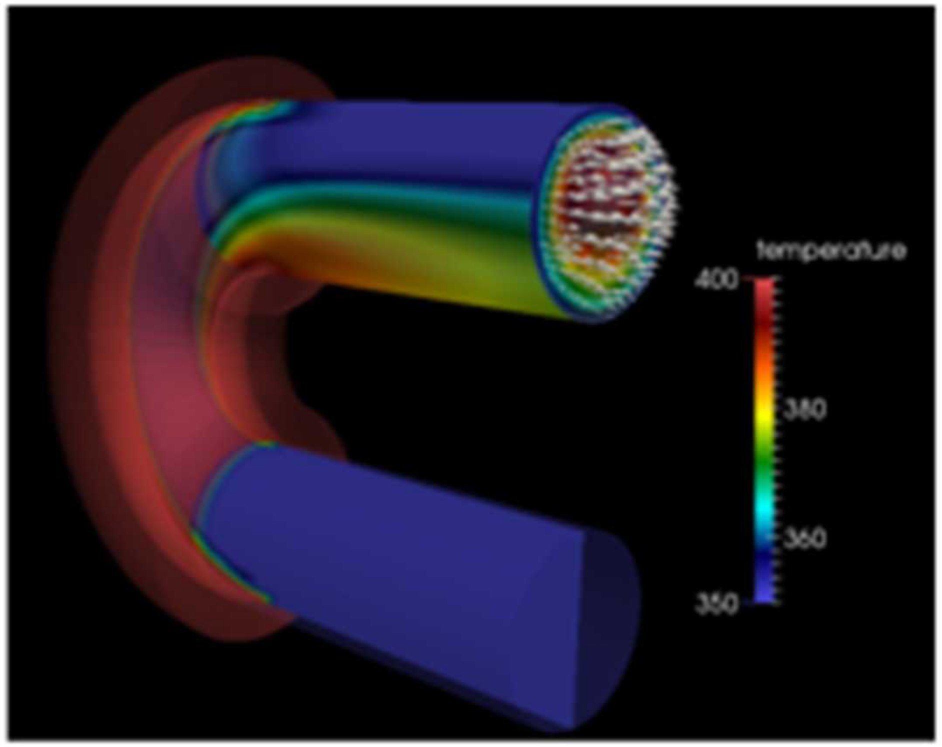
# Nalu

- www.github.com/spdomin/Nalu
- STK based
- Trilinos solvers
- scaling >500k cores

- prototype Kokkos assembly



**2D/3D sliding/overset mesh**




**multiphysics CHT**

# Existing Assembly

```
std::vector<double> lhs, rhs;
for ( auto && bptr : elem_buckets) {
    stk::mesh::Bucket & b = *bptr;

    std::vector<double> bucket_local_data(b.data_size());
    lhs.resize(...); rhs.resize(...);

    gather_data(b, bucket_local_data);

    const stk::mesh::Bucket::size_type num_elems = b.size();
    for ( stk::mesh::Bucket::size_type k = 0 ; k < num_elems ; ++k ) {
        stk::mesh::Entity elem = b[k];

        compute_kernel(elem, bucket_local_data, lhs, rhs);

        matrix.sum_into(elem, lhs, rhs);

    }
}
```

# Threading Issues

- local storage
  - **preallocated storage**

```
std::vector<double> bucket_local_data(b.data_size());
lhs.resize(...); rhs.resize(...);
```

- bucket size
  - **hierarchical parallelism**
- write conflicts
  - **atomics**

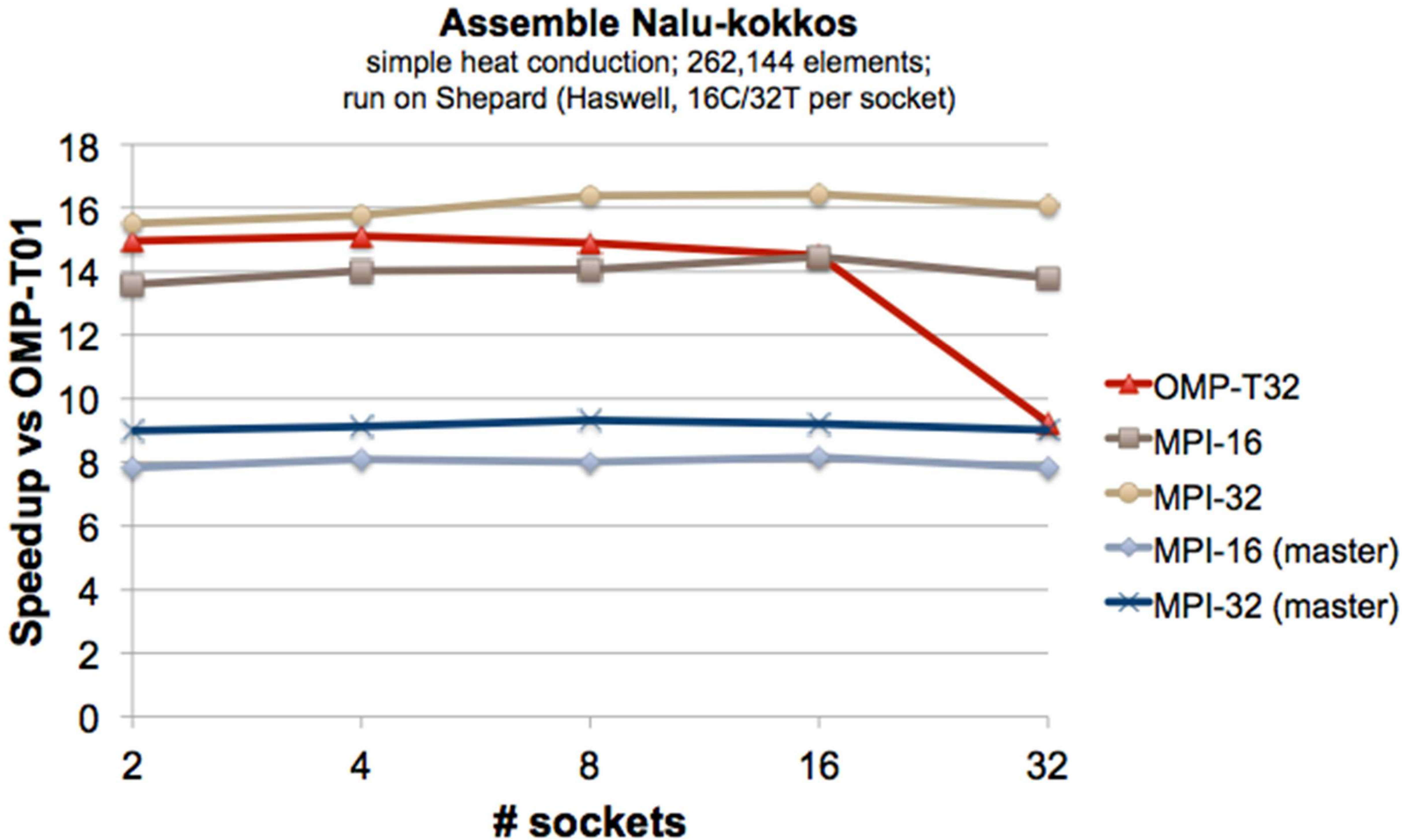
```
matrix.sum_into(elem, lhs, rhs);
```

- size of mesh data
  - **high bandwidth memory for scratch space**

# Kokkos Version

```
const int bytes_per_team = SharedMemView<double *>::shmem_size(team_data_size());
const int bytes_per_thread = SharedMemView<double *>::shmem_size(thread_data_size());
auto team_exec = get_team_policy(elem_buckets.size(), bytes_per_team, bytes_per_thread);

Kokkos::parallel_for("Alg::execute", team_exec, [&] (const DeviceTeam & team) {
  stk::mesh::Bucket & b = *elem_buckets[team.league_rank()];
  const stk::mesh::Bucket::size_type num_elems = b.size();

  SharedMemView<double*> bucket_local_data(team.team_shmem(), b.team_data_size());
  gather_data(b, bucket_local_data);

  SharedMemView<double*> lhs, rhs;
  lhs = Kokkos::subview(
    SharedMemView<double**>(team.team_shmem(), team.team_size(), lhsSize),
    team.team_rank(), Kokkos::ALL());
  rhs = Kokkos::subview(
    SharedMemView<double**>(team.team_shmem(), team.team_size(), rhsSize),
    team.team_rank(), Kokkos::ALL());
  team.team_barrier();

  Kokkos::parallel_for(Kokkos::TeamThreadRange(team, num_elems), [&] (const size_t k) {
    const stk::mesh::Entity elem = b[k];

    compute_kernel(elem, bucket_local_data, lhs, rhs);

    matrix.sum_into(elem, lhs, rhs);
  });
});
```

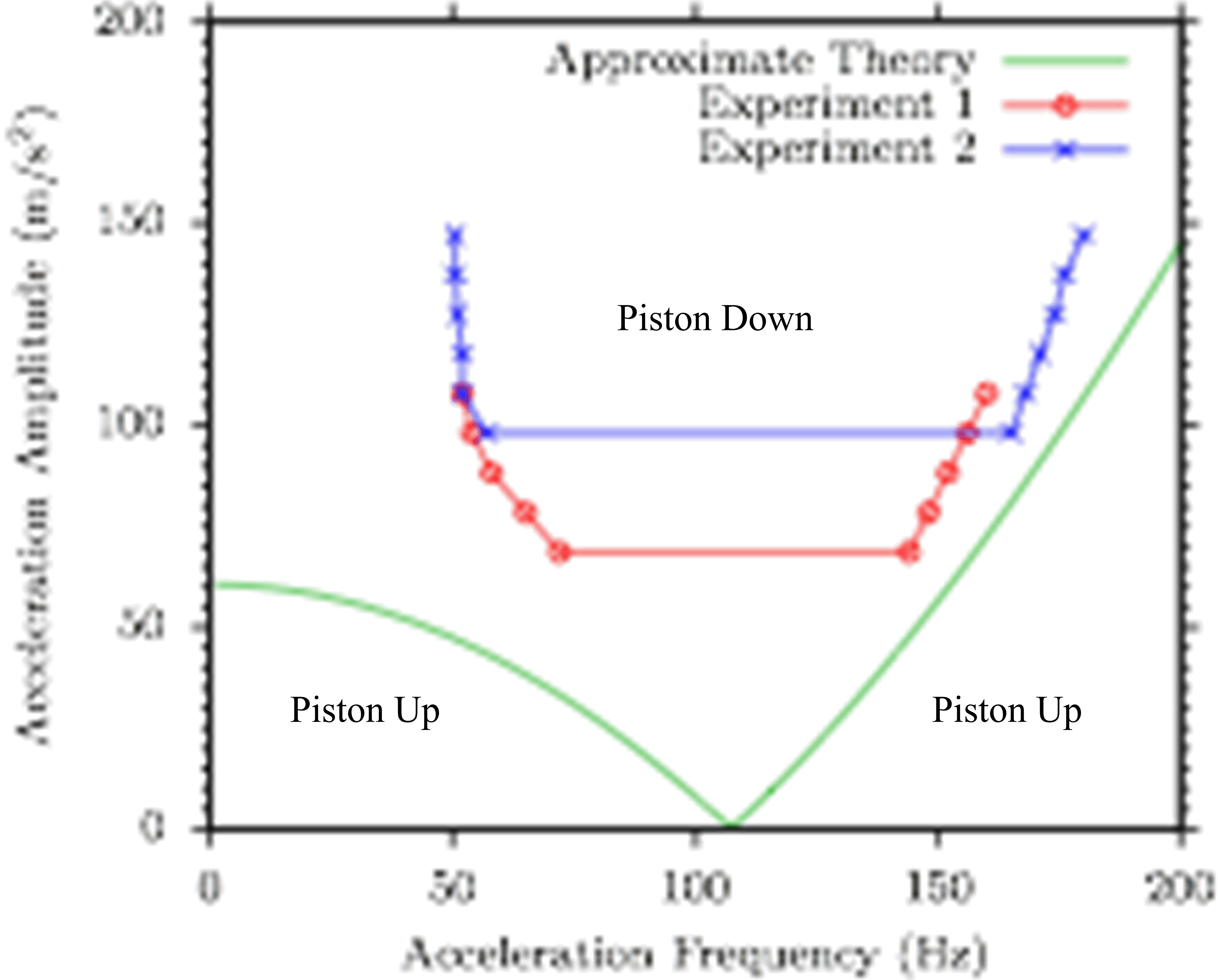
# Thread Scaling



# Conclusion

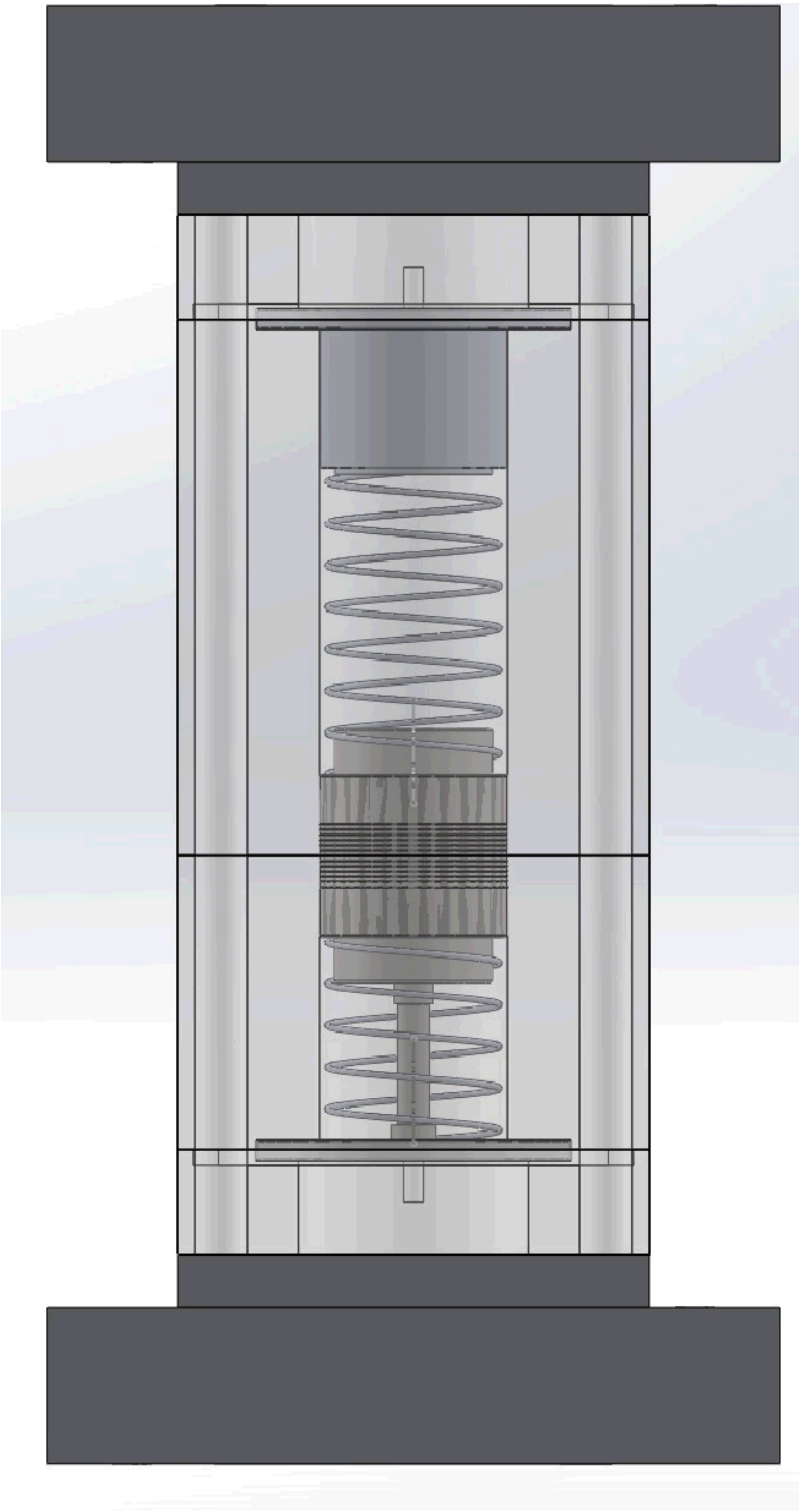
- Sierra Mechanics
- Piston–fluid system
- Next-generation platforms

# Experiments

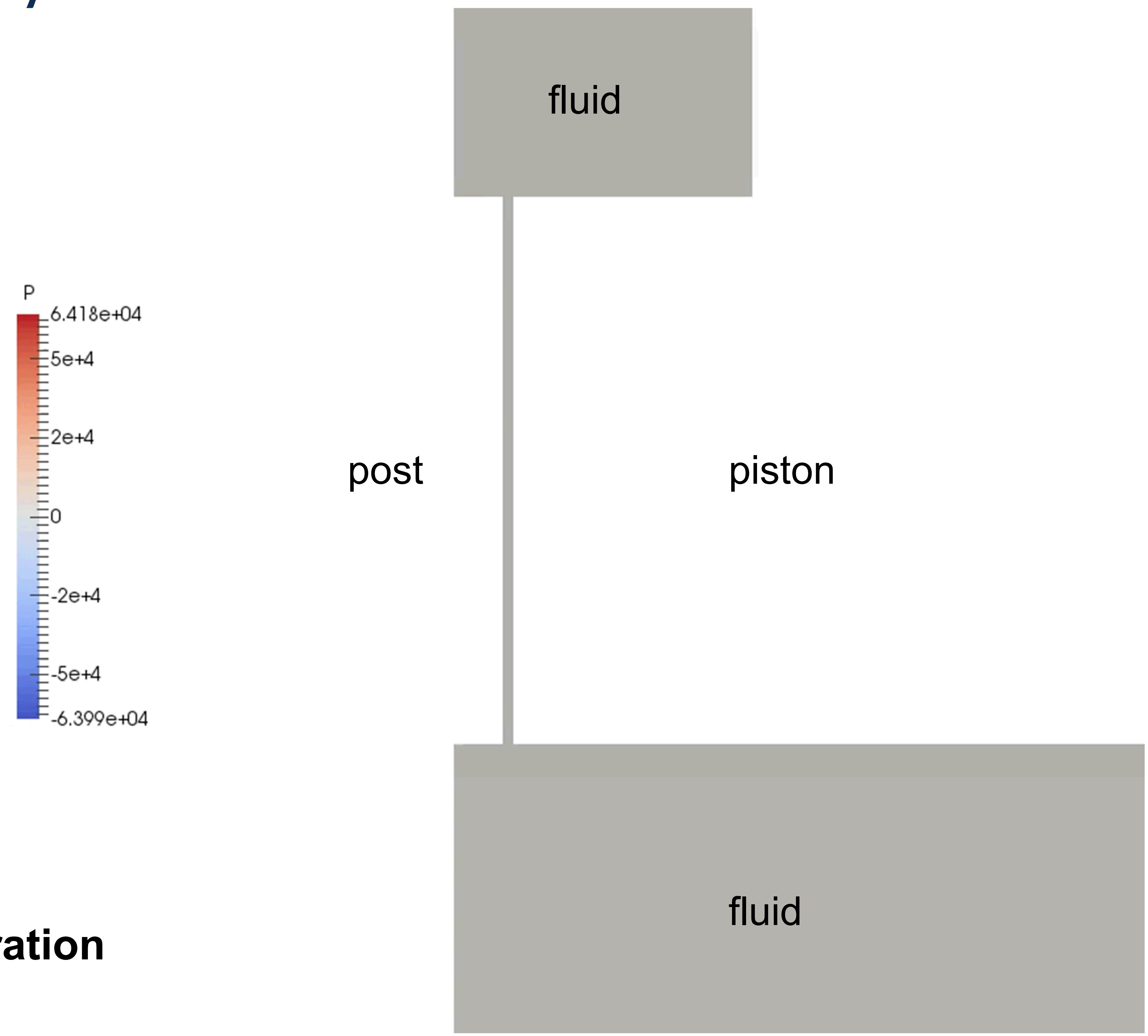


# Conclusions and Future Work

- Reduced-order model
- Full NS stimulation
- Preliminary experiments
- Dual-spring experiment that eliminates stops

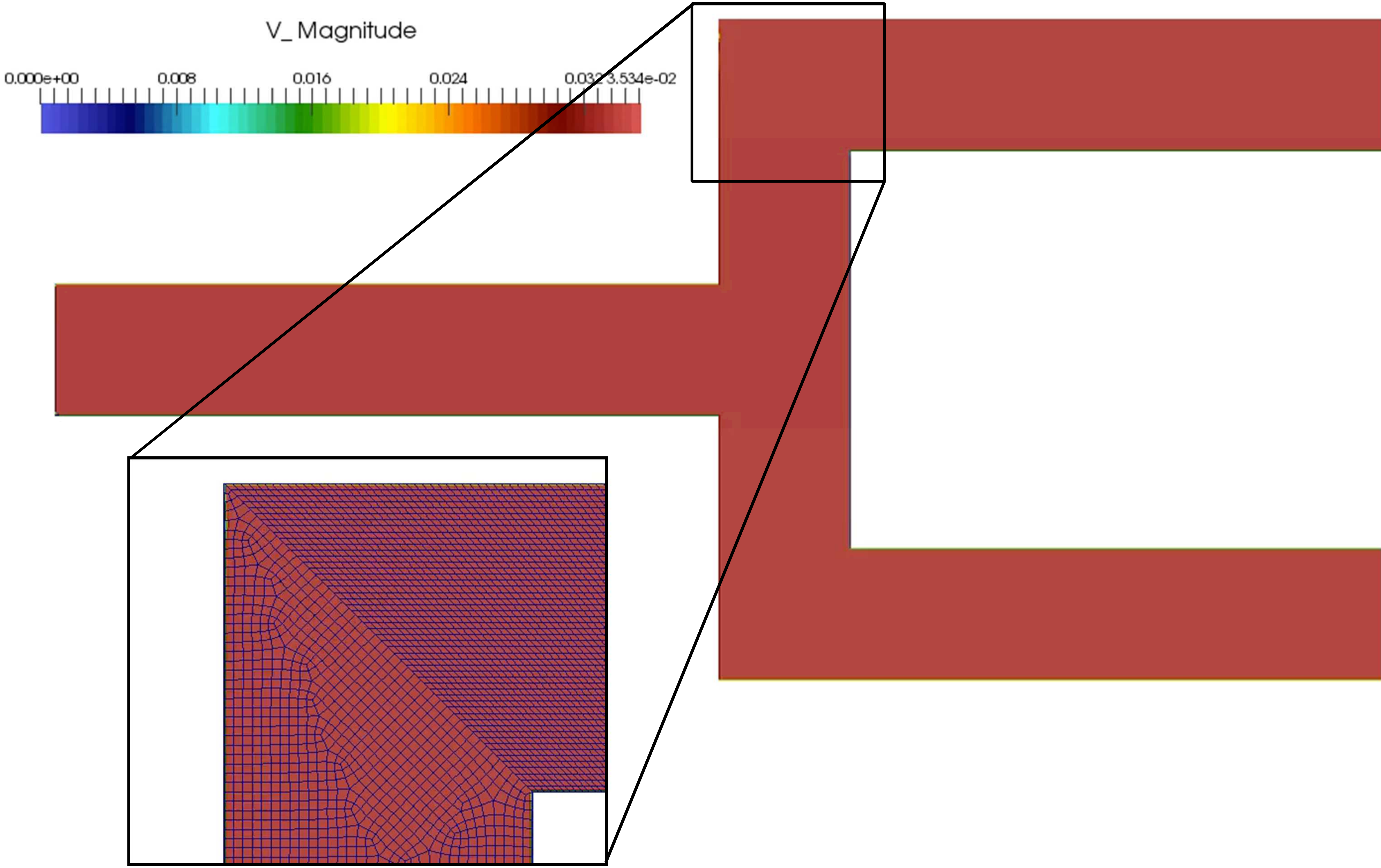


# Piston System

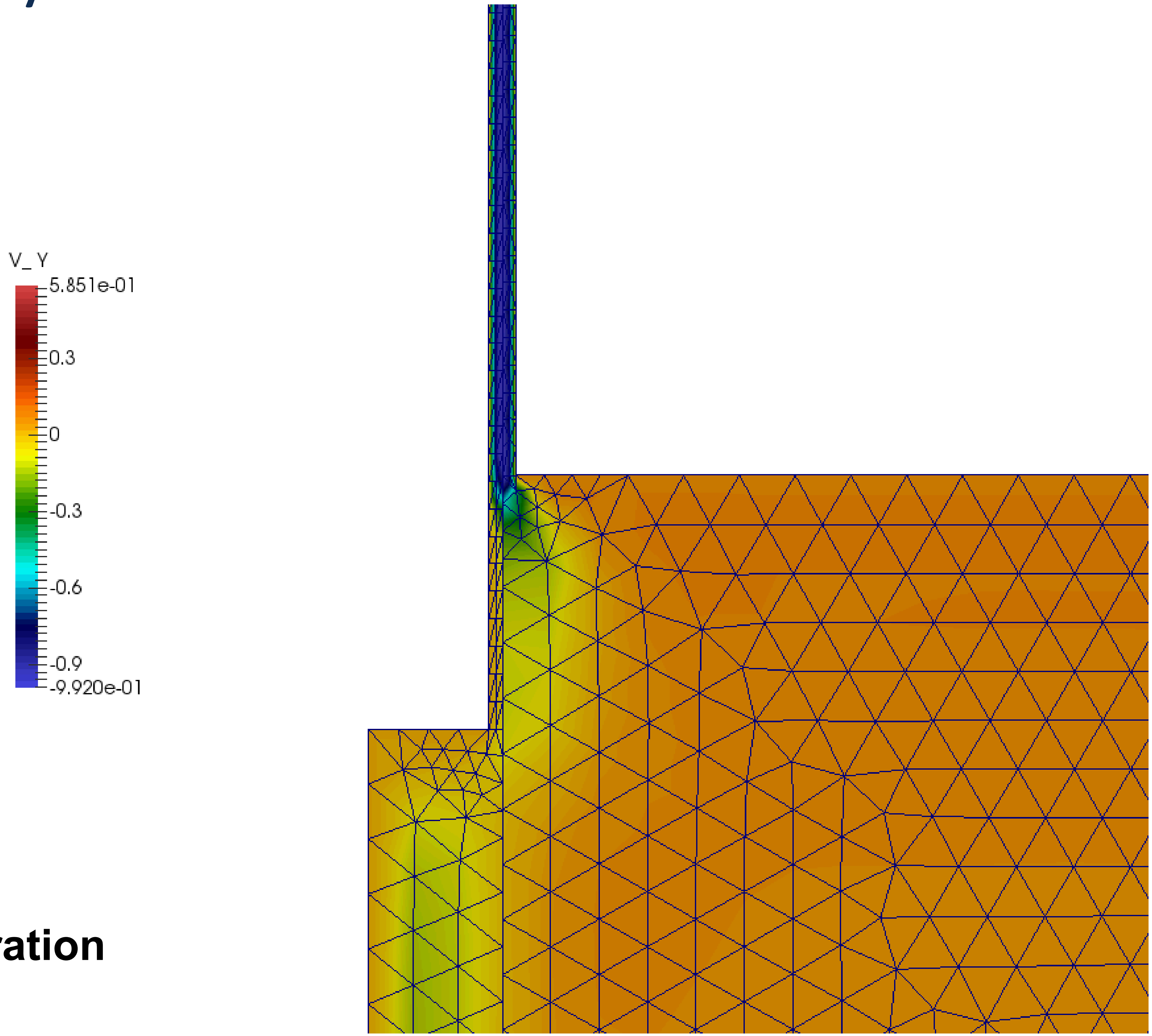



**10 g acceleration**
**100 Hz**

# Split-duct flow



# Piston System




**10 g acceleration**
**100 Hz**

# DG-style Numerical Fluxes