Numerical modeling of the submicrosecond solidification of materials undergoing dynamic compression

SSGF/LRGF Program Review
Outgoing Fellow Talk (Unlimited Audience)
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Q: How do we determine the equilibrium phase boundaries of materials at extreme P and T?

- A: Hold material at specific P and T until equilibrium phase develops

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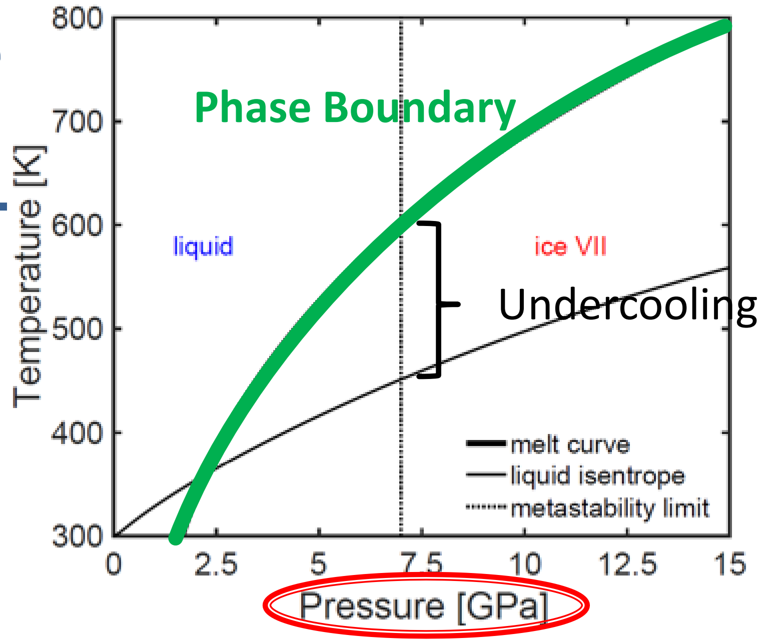
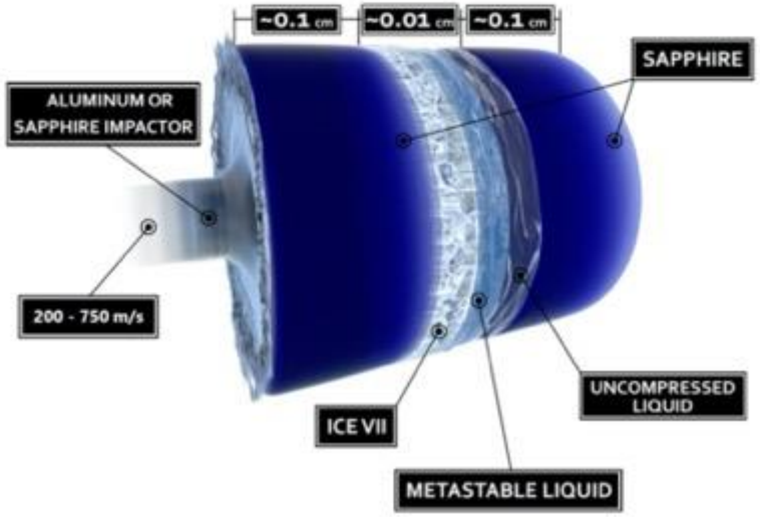
- A: Hold material at specific P and T until equilibrium phase develops

- Extreme P and T achieved using dynamic compression
  - — Overdriven past phase boundary
  - — Equivalent cooling rate: $\approx 10^9$ K/s
  - — P and T achieved for very short periods of time ($\leq \mu$s)
  - — Disallows sufficient time for true equilibrium phase to be reached

- Solution: Study nonequilibrium phase transition kinetics
  - — Deconvolve true equilibrium behavior of materials
  - — Determine phase boundaries

- Focus: Liquid water−ice VII phase transition

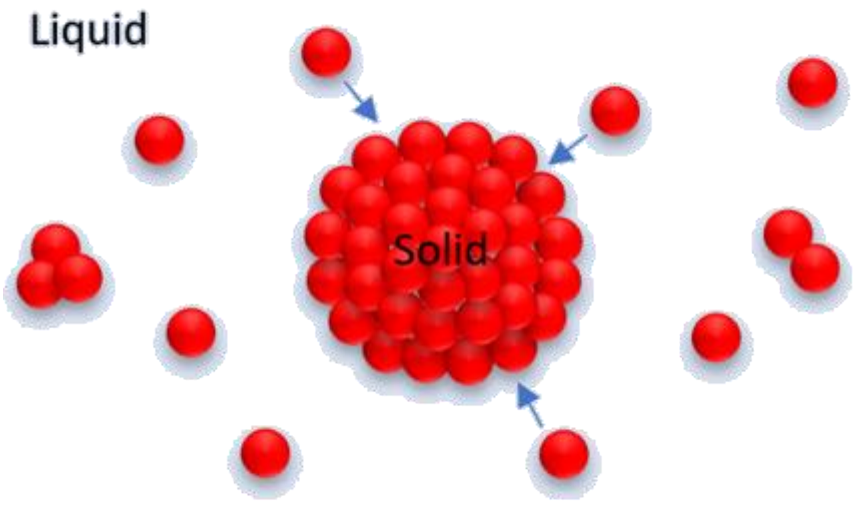




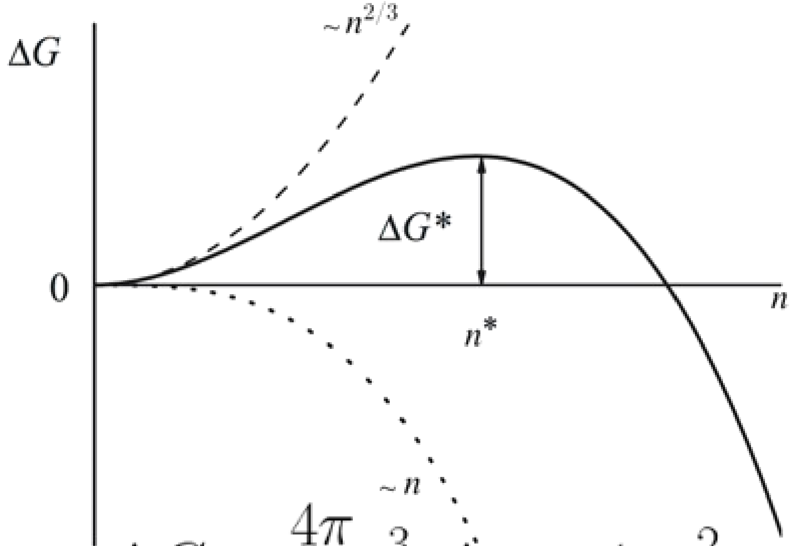
Dynamic-Compression Experiment (Impactor)

The transition to solid phase occurs through the nucleation and growth of solid clusters [1,2]

Solid clusters nucleate and grow from attachment of liquid molecules

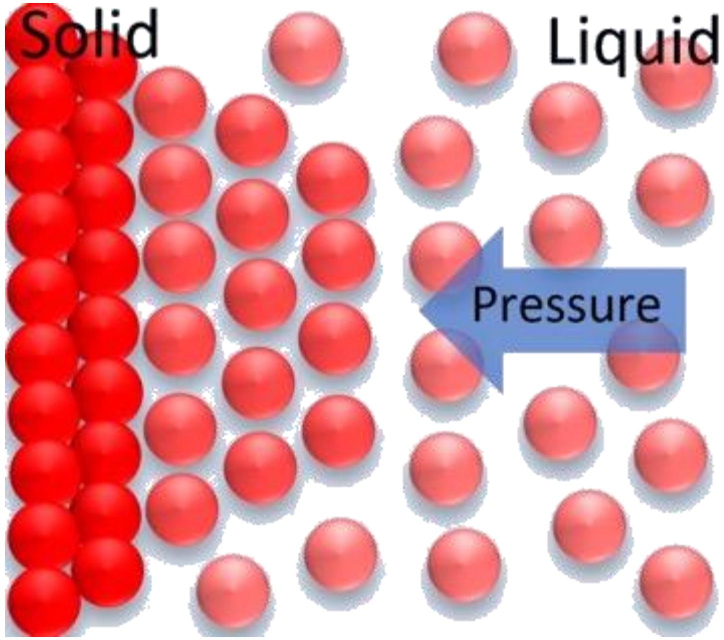


For solid clusters to nucleate, an energy barrier must be overcome
(Prevents immediate transition -> Kinetics)



$$\Delta G = \frac{4\pi}{3} r^3 \rho \Delta\mu + 4\pi r^2 \sigma$$
$$= n\Delta\mu + A\sigma$$

Under dynamic compression (high *P* and *Δμ*), cluster growth is rapid [3]



[1] D. Kashchiev, Nucleation: Basic Theory with Applications, 1st Edition, Butterworth-Heinemann, Burlington, MA, 2000, Ch. 3, 9-10.
[2] P. C. Myint, J. L. Belof, Rapid freezing of water under dynamic compression, Journal of Physics: Condensed Matter 30 (2018) 1-29.
[3] L. V. Mikheev, A. A. Chernov, Mobility of a diffuse simple crystal--melt interface, Journal of Crystal Growth 112 (1991) 591-596.

Hierarchy of Phase-Transition-Kinetics Modeling

Non-Equilibrium Molecular Dynamics

- Closest to natural phenomena
- Computationally expensive = Limited in time and length scales

Zel'dovich–Frenkel Cluster Kinetics (Non-steady state) ← This Research

Steady-State CNT
+ First-Principles Transience
(Becker–Döring Equations)

Steady-State CNT + Empirical Transient Term ← Myint et al. 2018

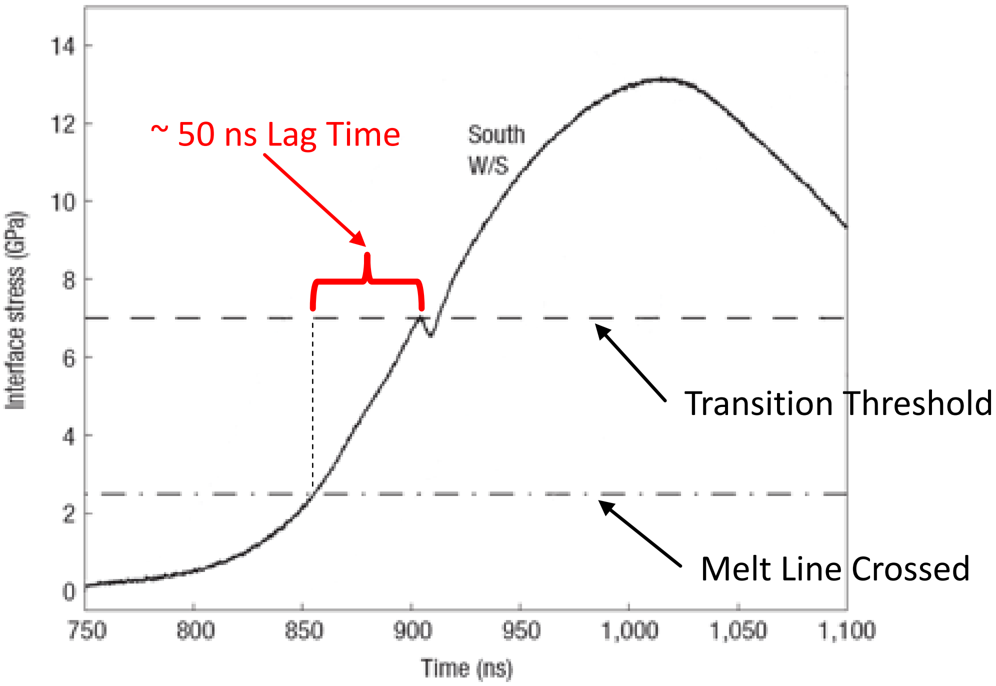
Used to model liquid water–ice VII transition

Steady-State Classical Nucleation Theory (CNT) ↔ Not always consistent ↔ **Experimental Measurements**

Zel'dovich—Frenkel numerical model calculates nucleation lag time without requiring transient empirical scaling parameter

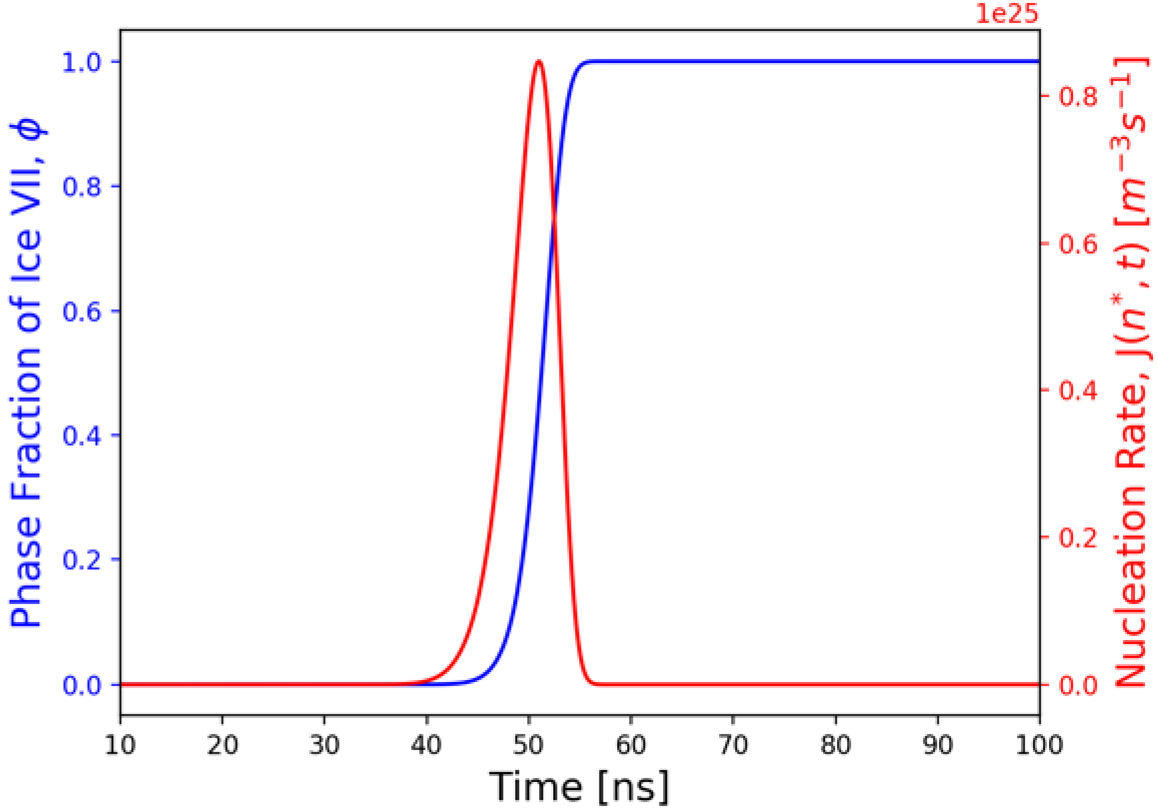
- Lag time: ≈ 50 ns
- Eliminates need for empirical scaling parameter needed (Myint et al. 2018 [1]) for transient behavior

From Dolan et al. 2007 Experiment



ZF numerical model

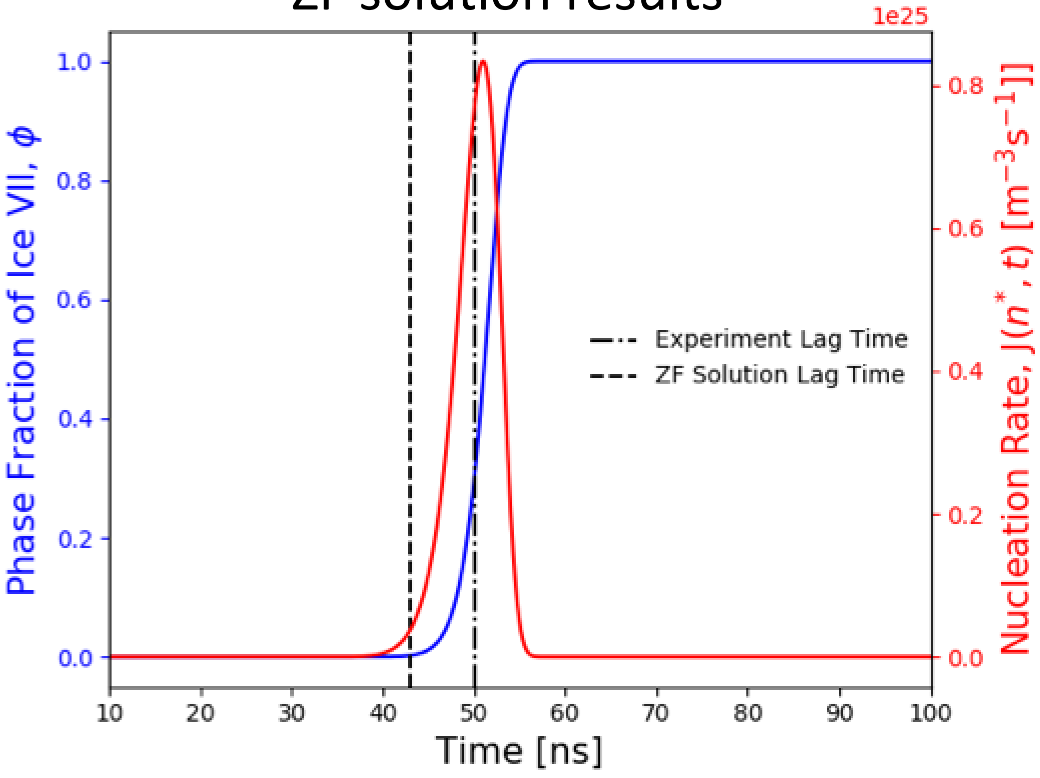
$$\frac{\partial f(n,t)}{\partial t} = -\frac{\partial J(n,t)}{\partial n} \qquad J(n,t) = -D^{+}(n,t) f_{\mathrm{eq}}(n;t) \frac{\partial}{\partial n}\left(\frac{f(n,t)}{f_{\mathrm{eq}}(n;t)}\right)$$



[1] P. C. Myint, A. A. Chernov, B. Sadigh, L. X. Benedict, B. M. Hall, S. Hamel, J. L. Belof, Nanosecond freezing of water at high pressures: Nucleation and growth near the metastability limit, Physical Review Letters 121 (15).

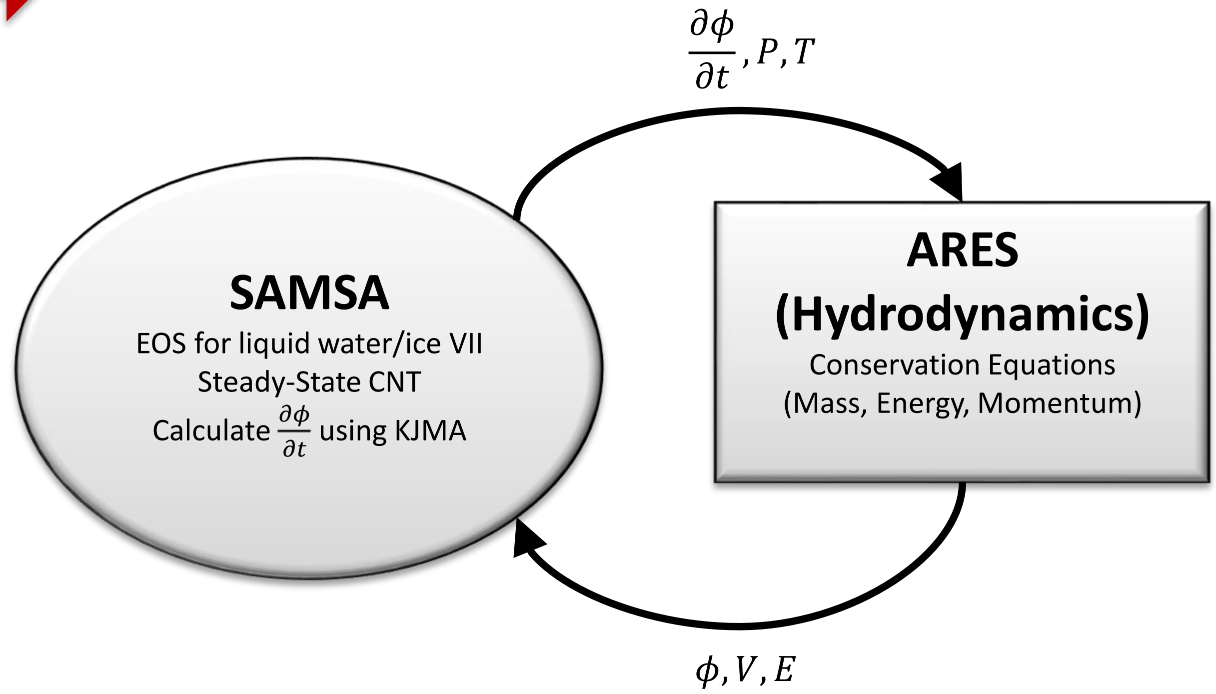
ZF solution accounts for transient kinetics, but there is still some deviation from experimental results

ZF solution results



Lag time is off by 5-10 ns

Need to account for hydrodynamics effects in simulations



Mass

$$\frac{D\rho}{Dt} = -\rho \nabla \cdot u$$

Momentum

$$\rho \frac{Du}{Dt} = -\nabla P(\phi)$$

Energy

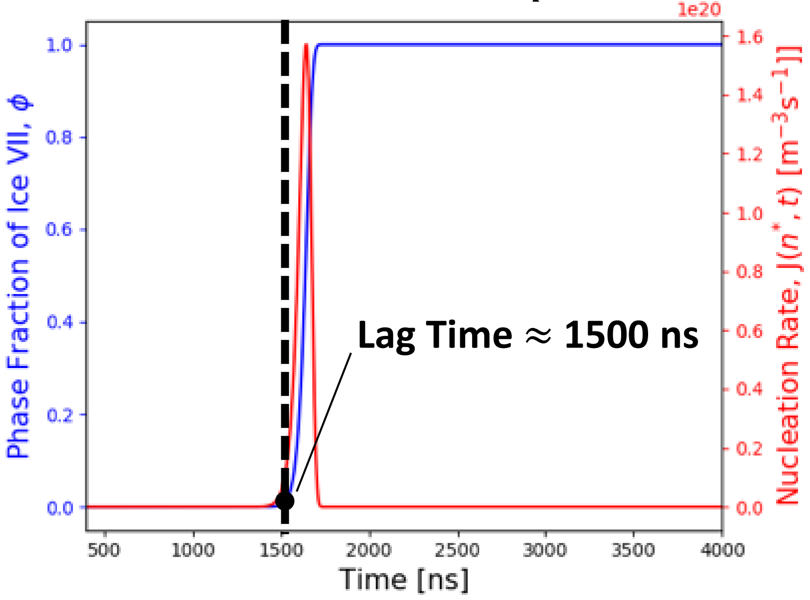
$$\rho \frac{DE}{Dt} = -P(\phi) \nabla \cdot u$$

Also, small amount of empirical refinement of σ model needed to closely match experiments

Depending on the compression timescale, the transition lag time after crossing melt line can vary by orders of magnitude

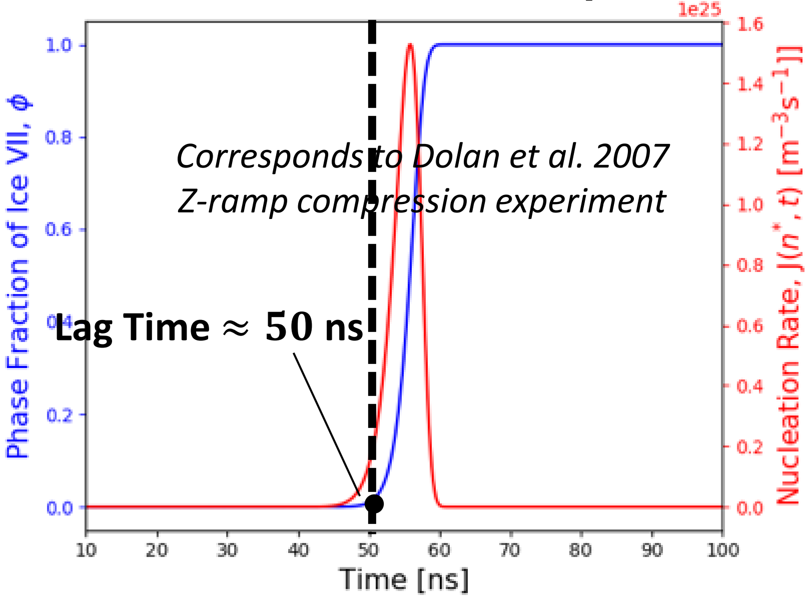
From ZF numerical model

Compression Timescale: τ_{comp} = 2000 ns (2 μs)



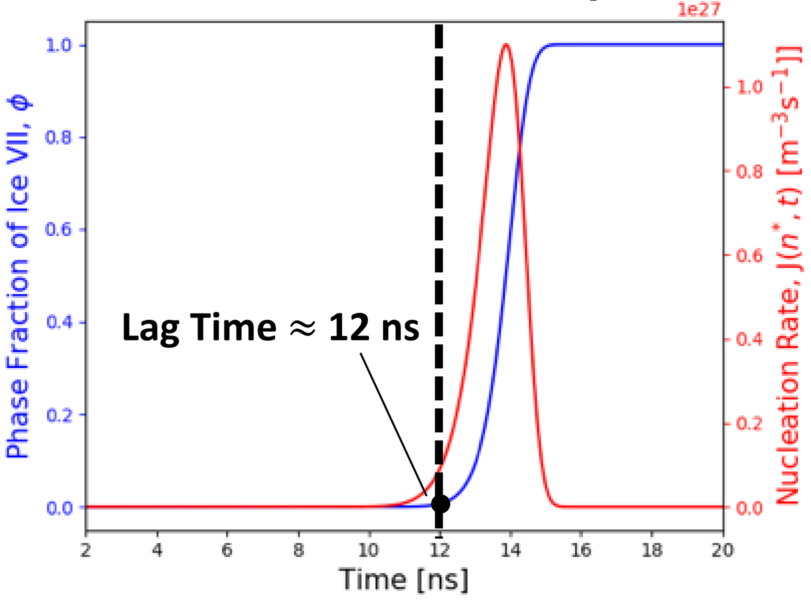
From ZF numerical model

Compression Timescale: τ_{comp} = 50 ns

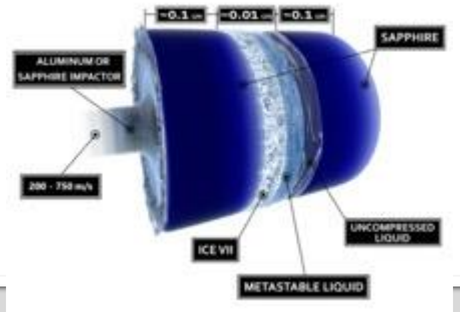


From ZF numerical model

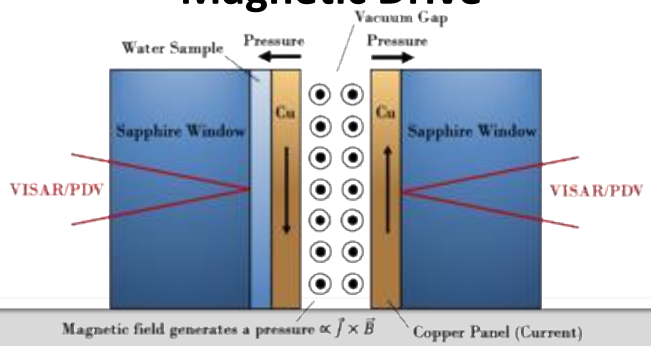
Compression Timescale: τ_{comp} = 10 ns



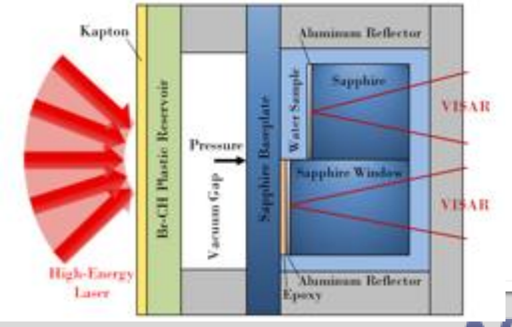
Gas-gun-driven Impactor



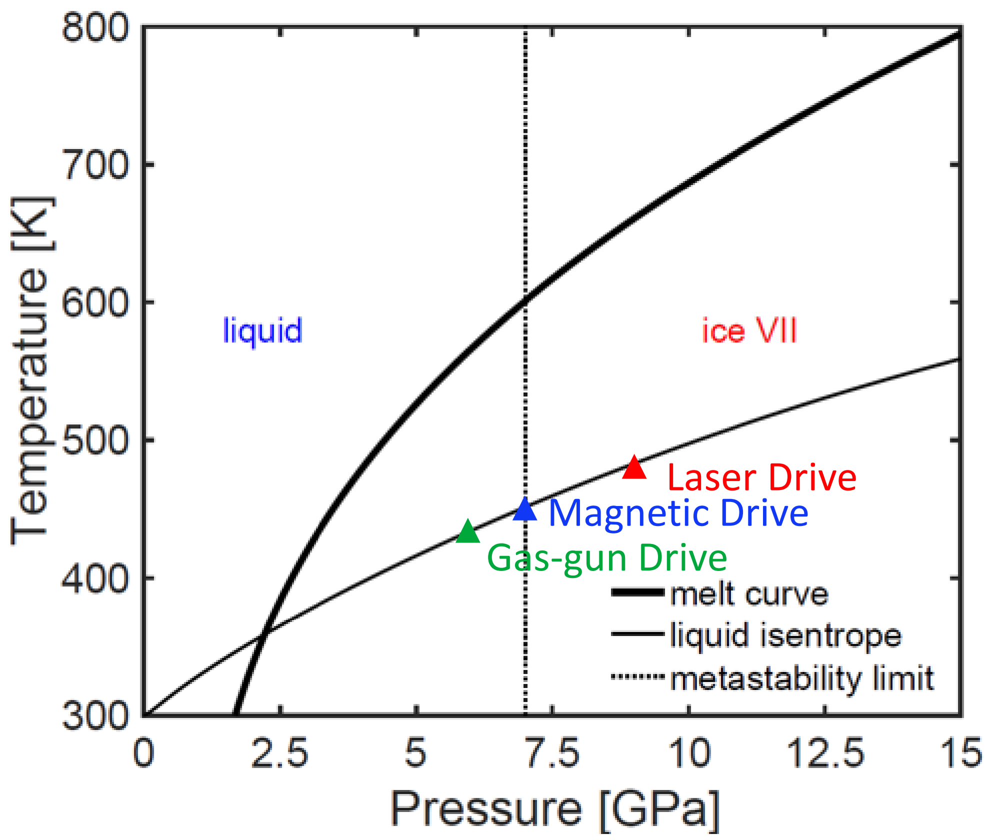
Magnetic Drive

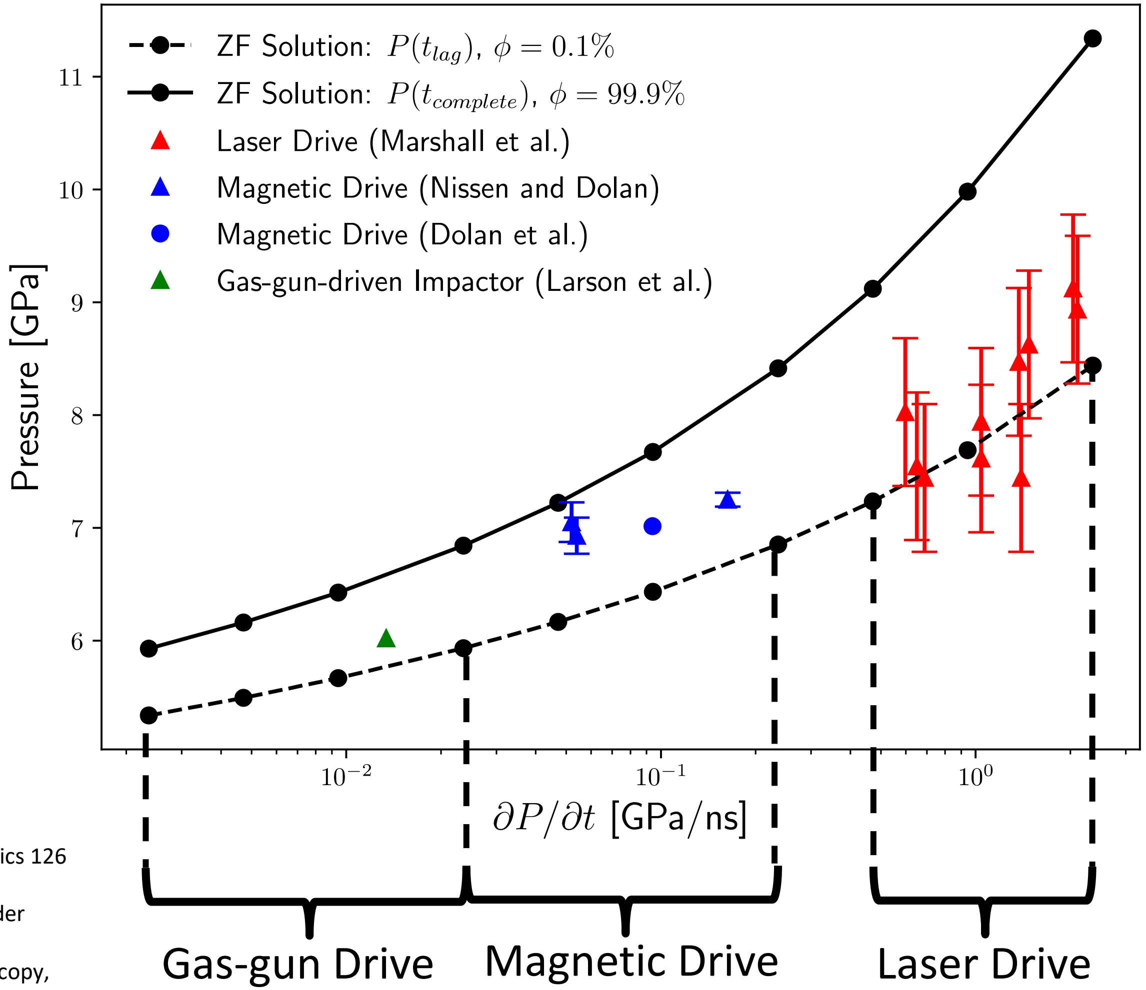


High-Energy Lasers



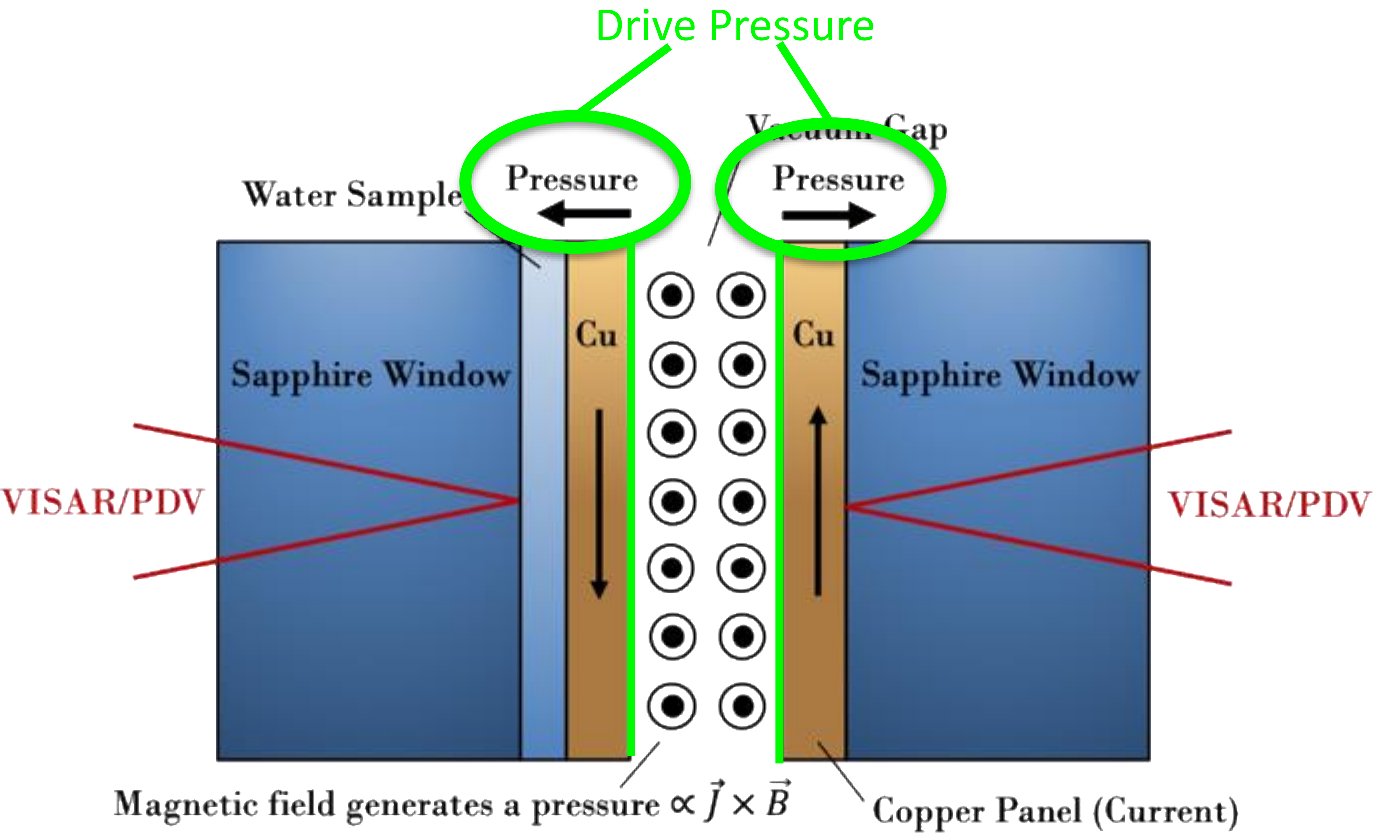
Transition pressure from simulations appears to be consistent with experiments conducted at a range of compression rates





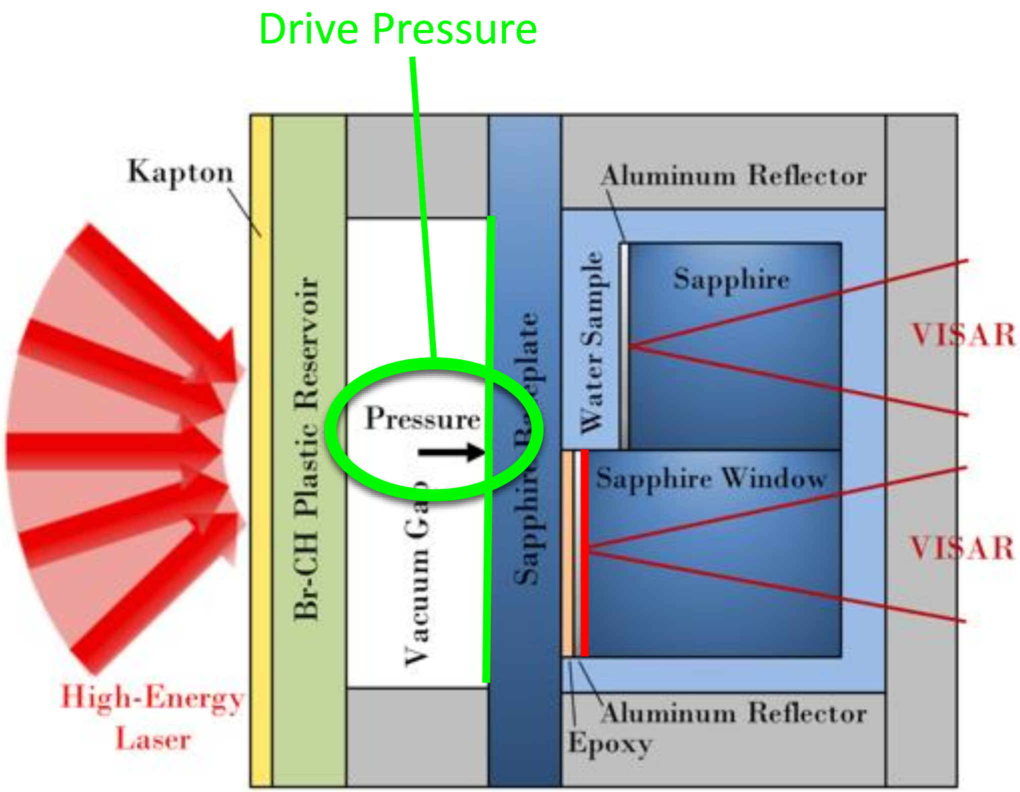
[1] E. J. Nissen, D. H. Dolan, Temperature and rate effects in ramp-wave compression freezing of liquid water, Journal of Applied Physics 126 (1) (2019) 015903.
[2] M. Marshall, M. Millot, D. Fratanduono, P. Myint, J. Belof, R. Smith, J. McNaney, Probing the metastability limit of liquid water under dynamic compression, 21st Biennial Conference of the APS Topical Group on Shock Compression of Condensed Matter, 64 (8).
[3] E. Larson, J. Mance, B. M. La Lone, M. Staska, R. Valencia, Fast temperature measurements using dispersive time-domain spectroscopy, (in preparation for publication)

Determining the drive pressure in dynamic-compression experiments is essential for performing forward hydrodynamics simulations



Magnetic-Drive Ramp-Wave Compression

(Nissen and Dolan Experimental Setup [1])

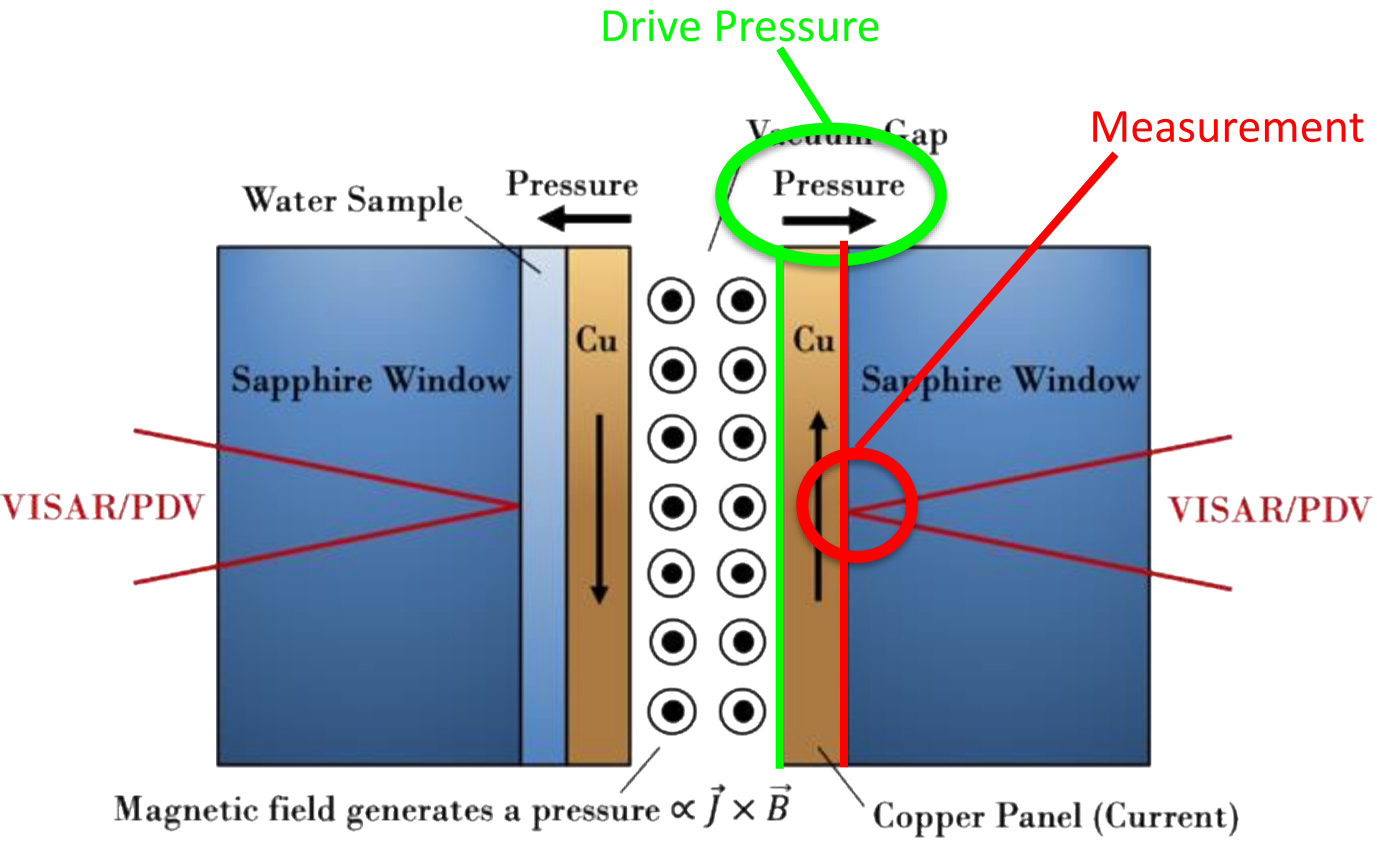


Laser-Drive Ramp-Wave Compression

(Marshall et al. Experimental Setup [2])

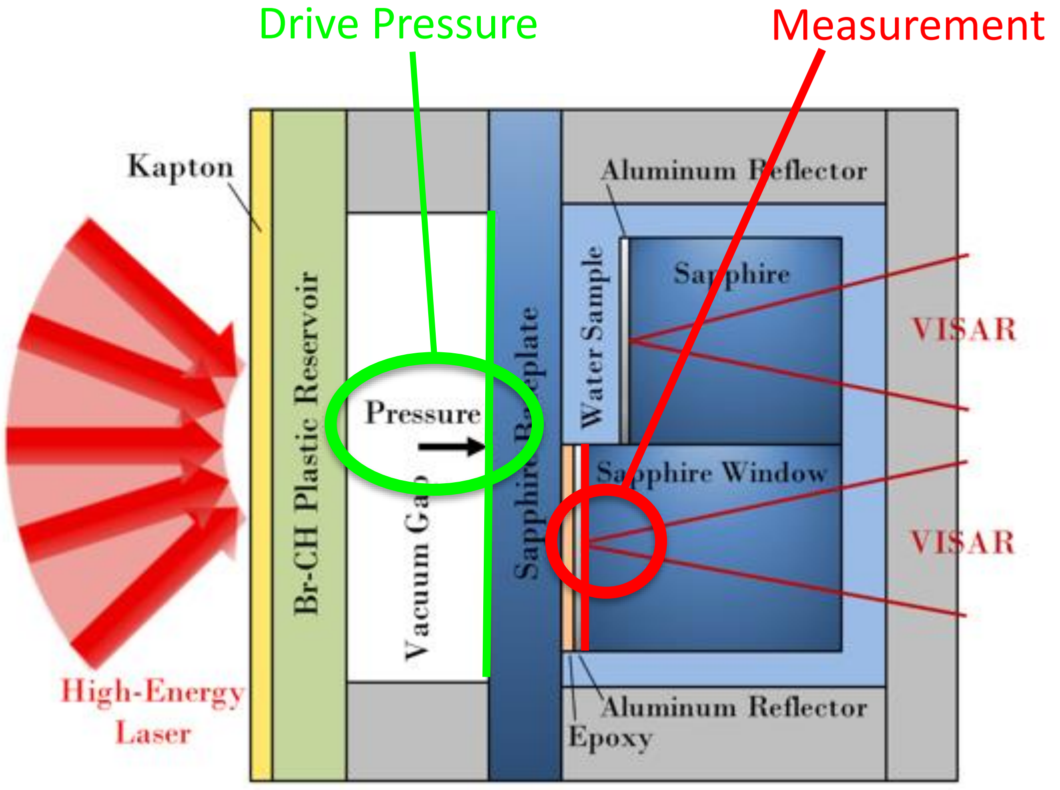
[1] E. J. Nissen, D. H. Dolan, Temperature and rate effects in ramp-wave compression freezing of liquid water, Journal of Applied Physics 126 (1) (2019) 015903.
[2] M. Marshall, M. Millot, D. Fratanduono, P. Myint, J. Belof, R. Smith, J. McNaney, Probing the metastability limit of liquid water under dynamic compression, 21st Biennial Conference of the APS Topical Group on Shock Compression of Condensed Matter, 64 (8).

In ramp-wave compression experiments, an inverse problem is created where experimental measurements must be used to determine the drive pressure



Magnetic-Drive Ramp-Wave Compression

(Nissen and Dolan Experimental Setup [1])

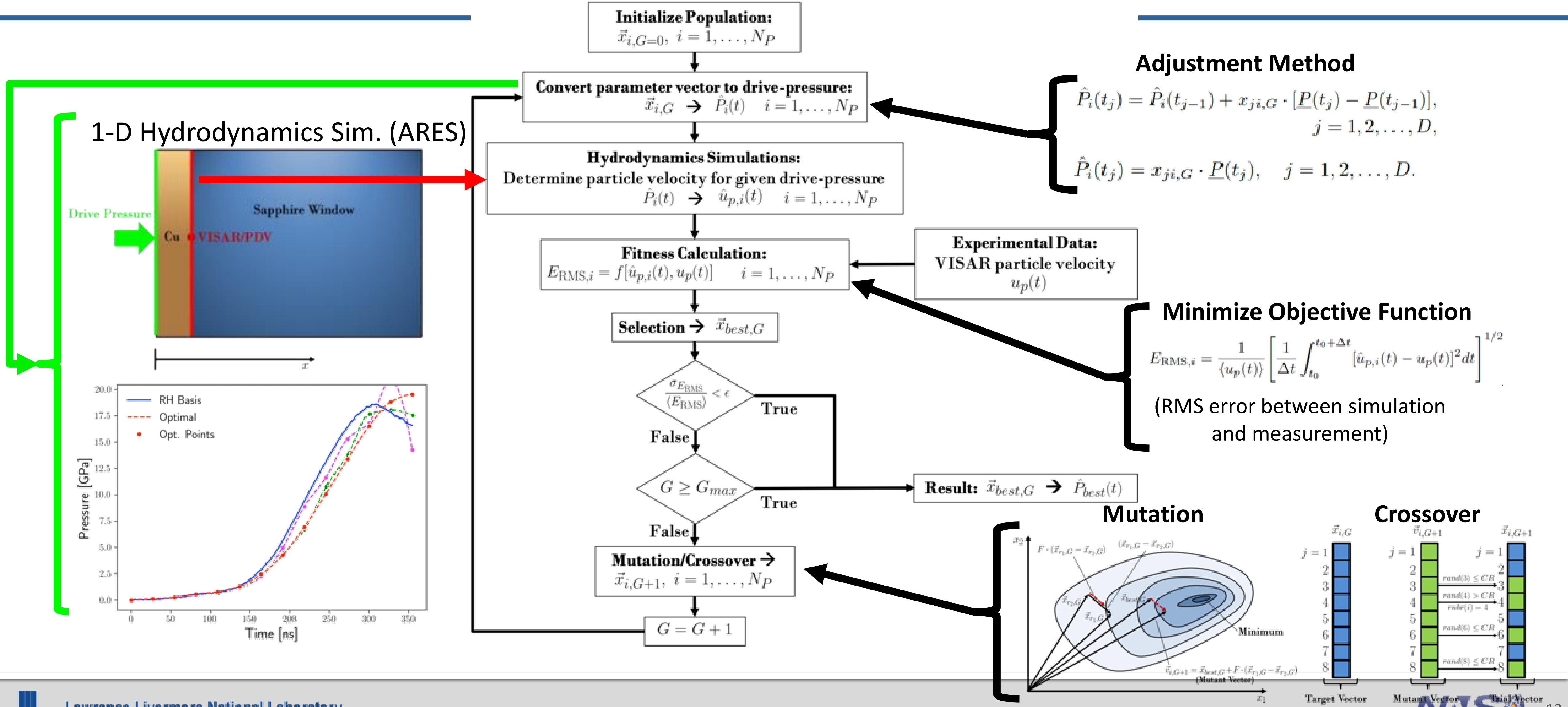


Laser-Drive Ramp-Wave Compression

(Marshall et al. Experimental Setup [2])

[1] E. J. Nissen, D. H. Dolan, Temperature and rate effects in ramp-wave compression freezing of liquid water, Journal of Applied Physics 126 (1) (2019) 015903.
[2] M. Marshall, M. Millot, D. Fratanduono, P. Myint, J. Belof, R. Smith, J. McNaney, Probing the metastability limit of liquid water under dynamic compression, 21st Biennial Conference of the APS Topical Group on Shock Compression of Condensed Matter, 64 (8).

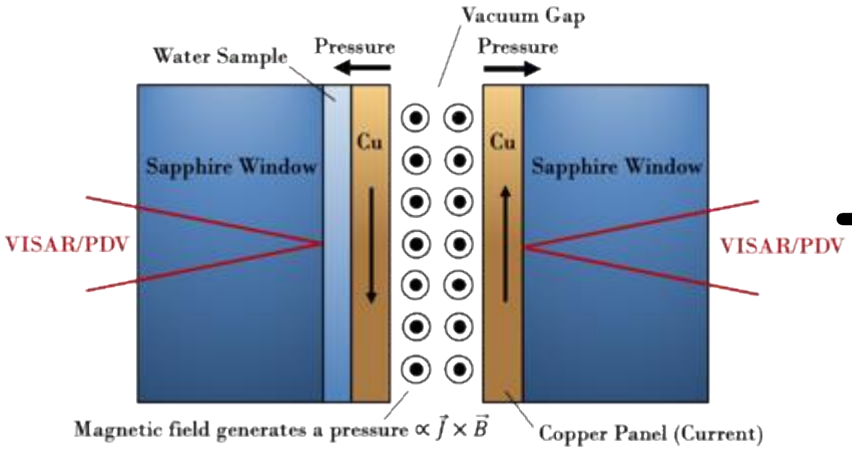
Overview of differential evolution algorithm as applied to drive-pressure optimization problem



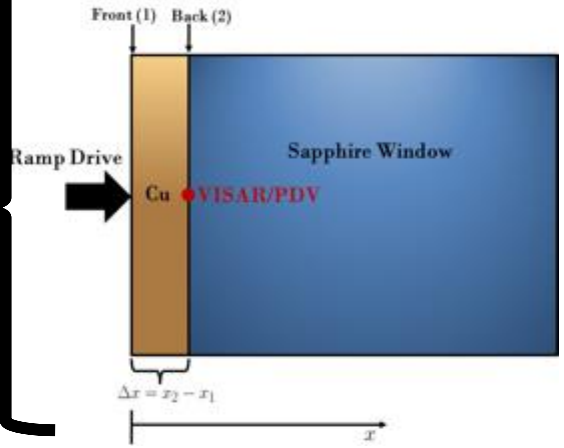
Drive-pressure optimization is applied to both magnetic-drive and laser-drive experiments to demonstrate applicability

Magnetic-Drive Ramp-Wave Compression

(Nissen and Dolan Experimental Setup)



1-D Hydrodynamics Simulations

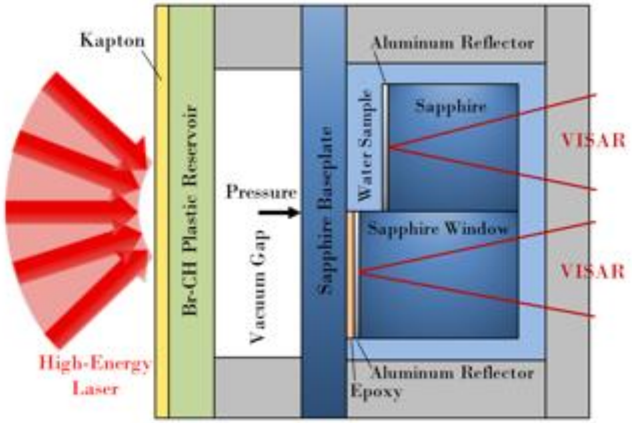


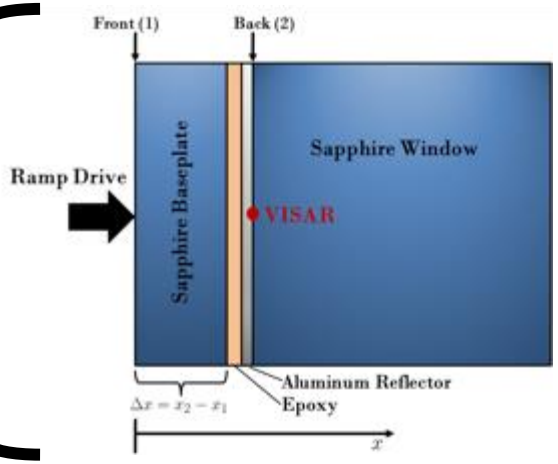
Experiments:

Exp. 1
Exp. 2
Exp. 3
Exp. 4
Exp. 5
Exp. 6

Laser-Drive Ramp-Wave Compression

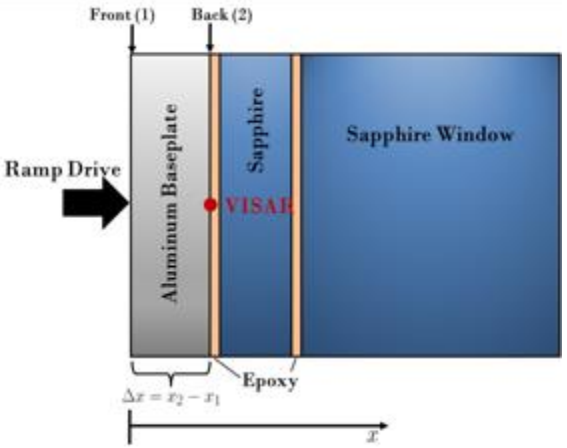
(Marshall et al. Experimental Setup)





Experiments:

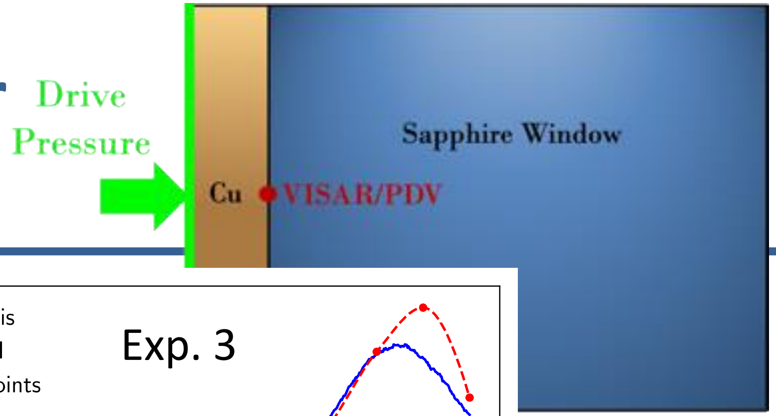
Exp. 29419
Exp. 31418
Exp. 31424

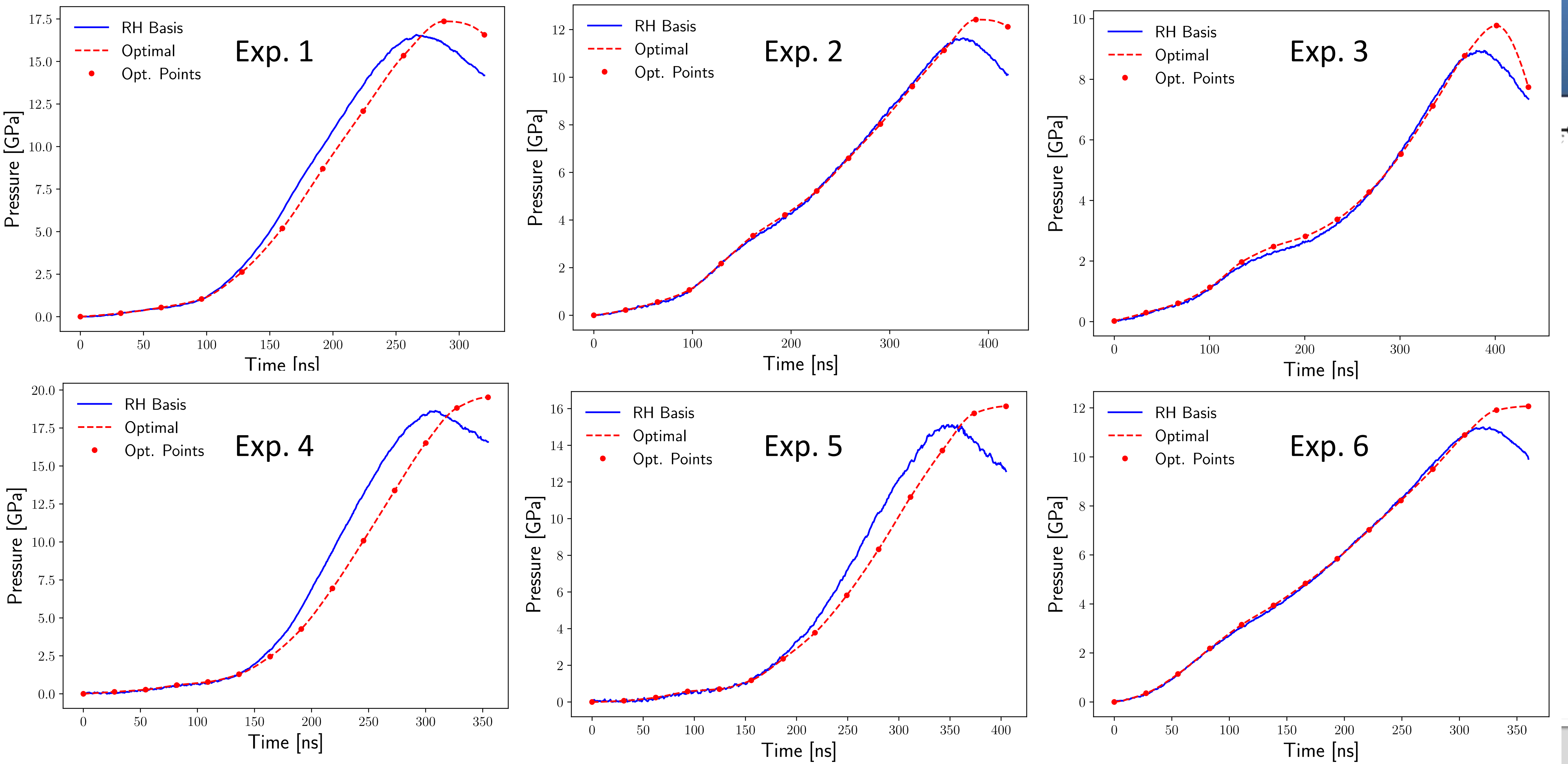


Experiments:

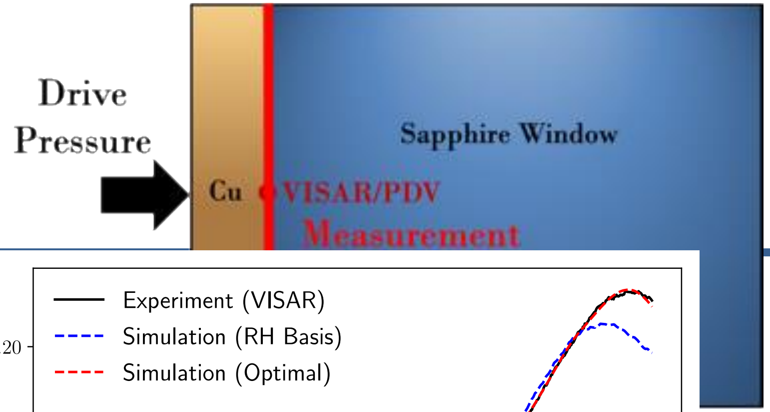
Exp. 88458

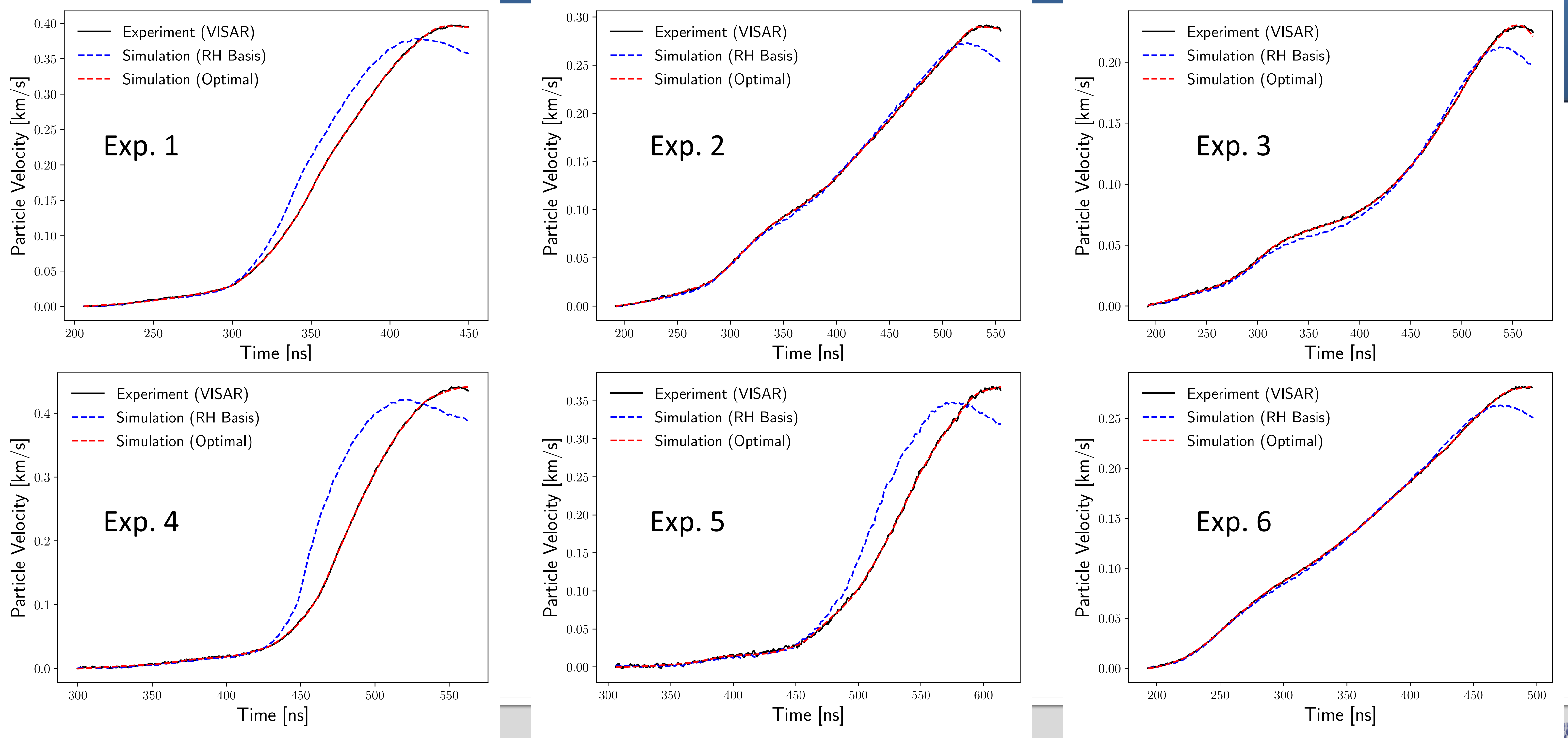
Optimization produces the following drive pressures for the magnetic-drive experiments of Nissen and Dolan



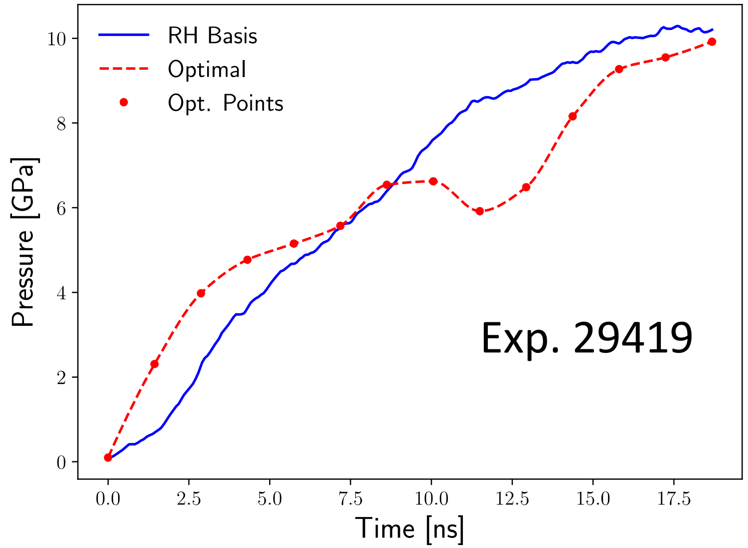


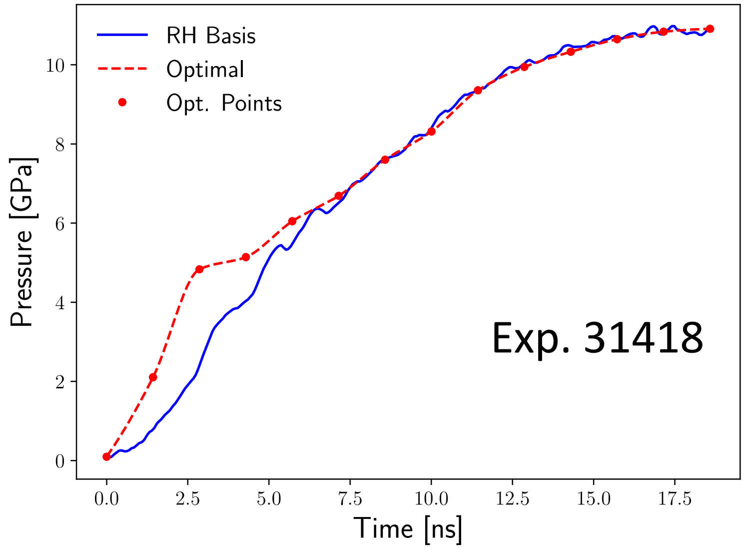
Drive-pressure optimization produces excellent agreement with experiment for magnetic-drive experiments of Nissen and Dolan

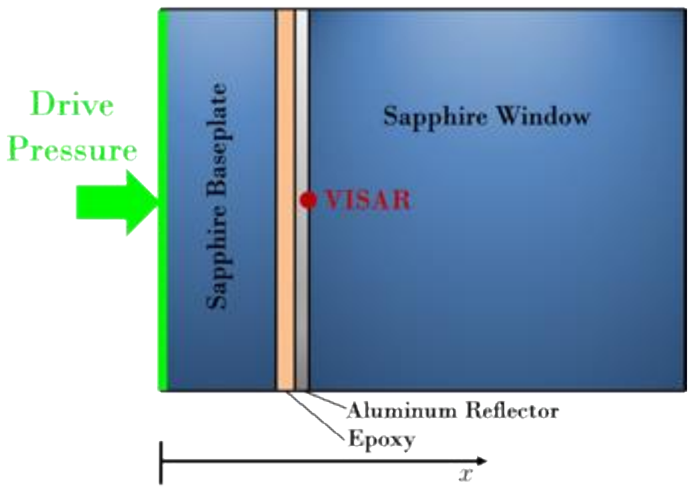


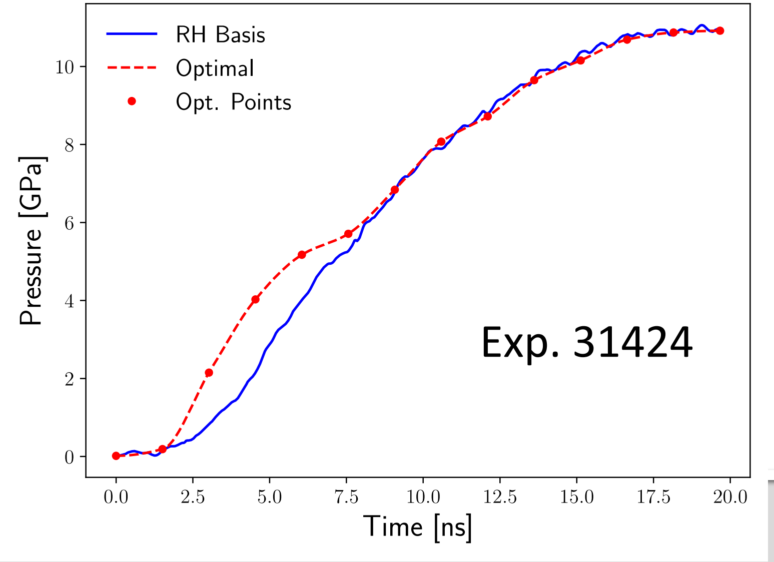


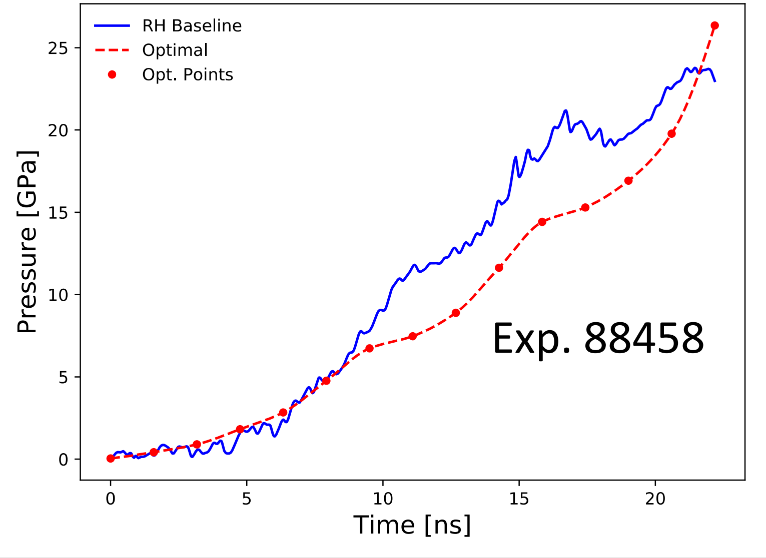
Optimization produces the following drive pressures for the laser-drive experiments of Marshall et al.



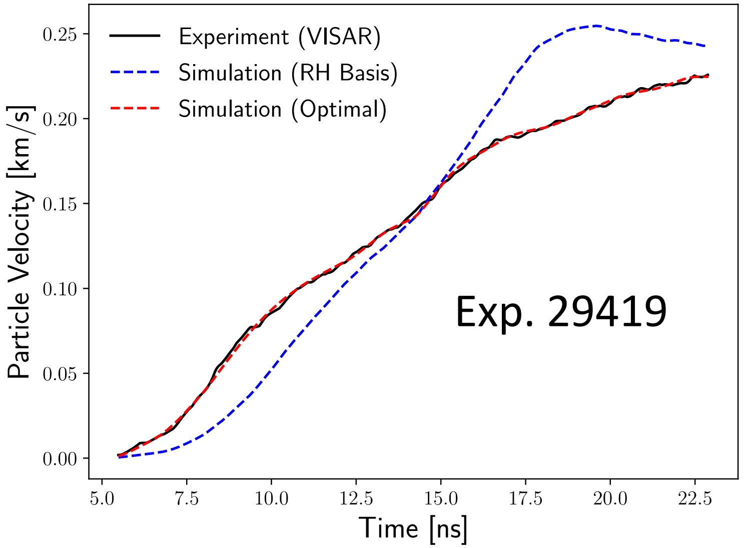


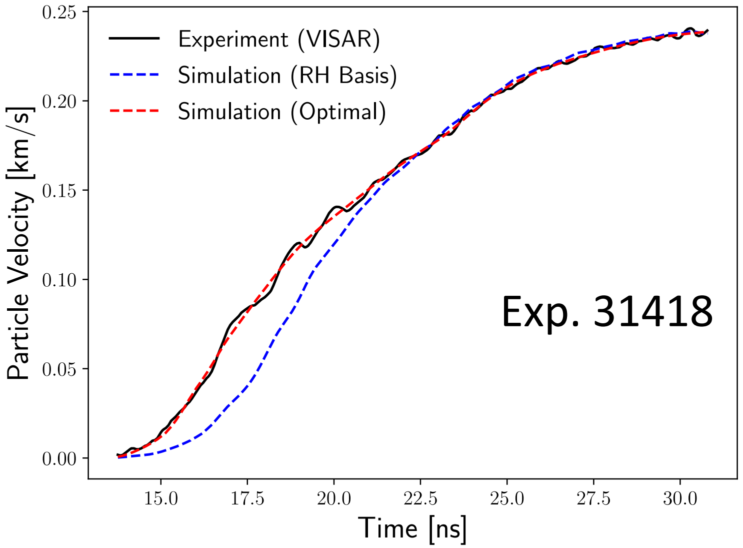


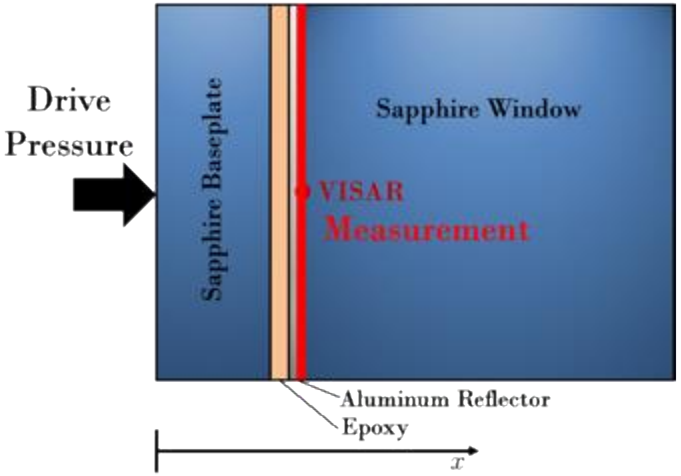


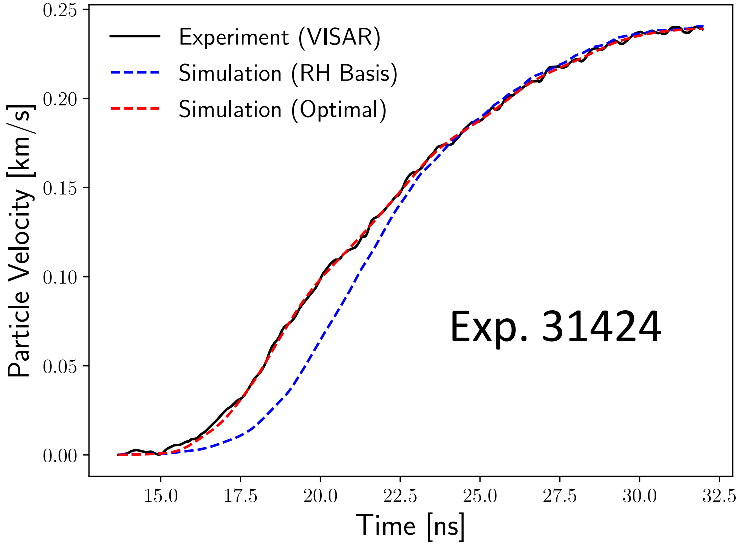


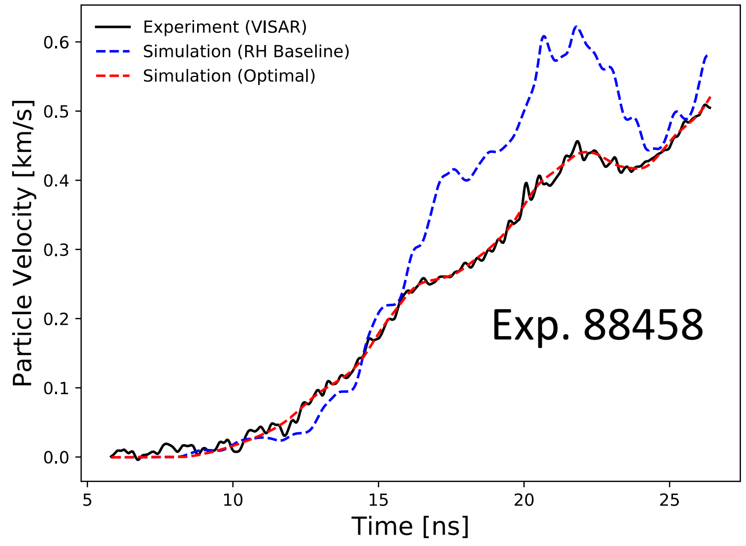
Drive-pressure optimization also produces excellent agreement with experiment for laser-drive experiments of Marshall et al.



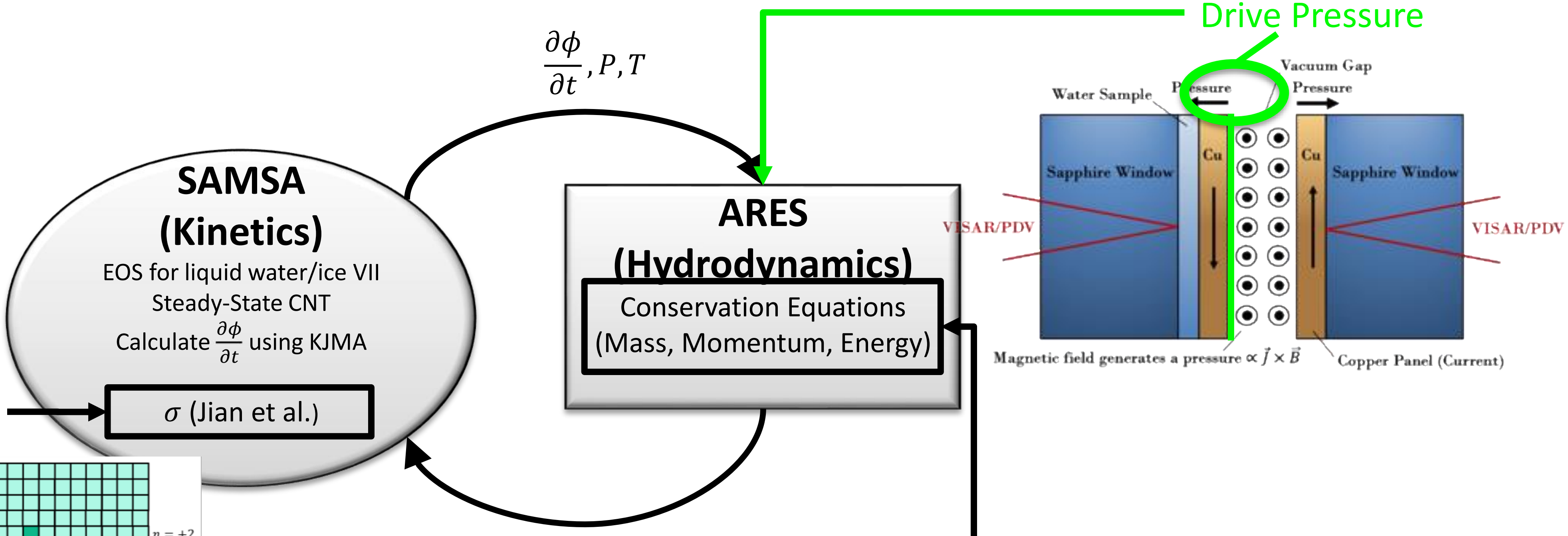




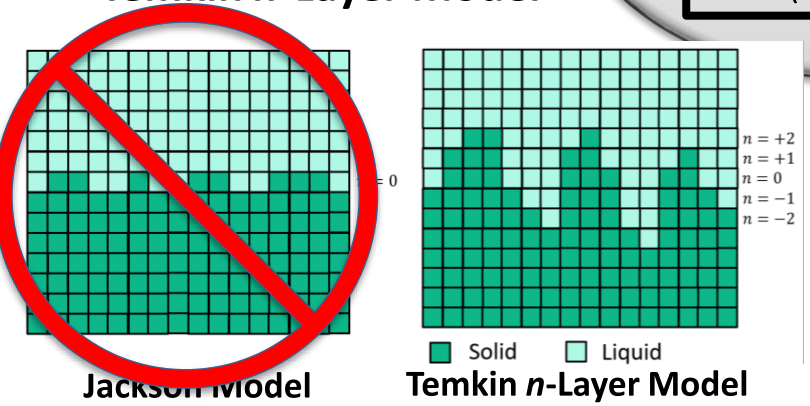




Forward simulations on water side can account for both phase transition kinetics and hydrodynamics



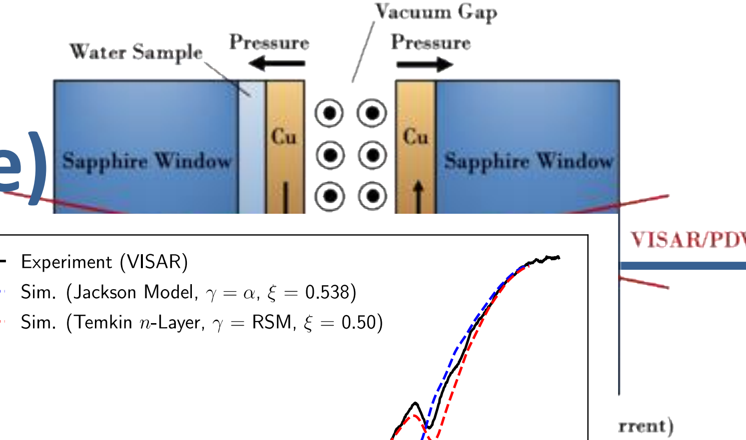
Temkin *n*-Layer Model

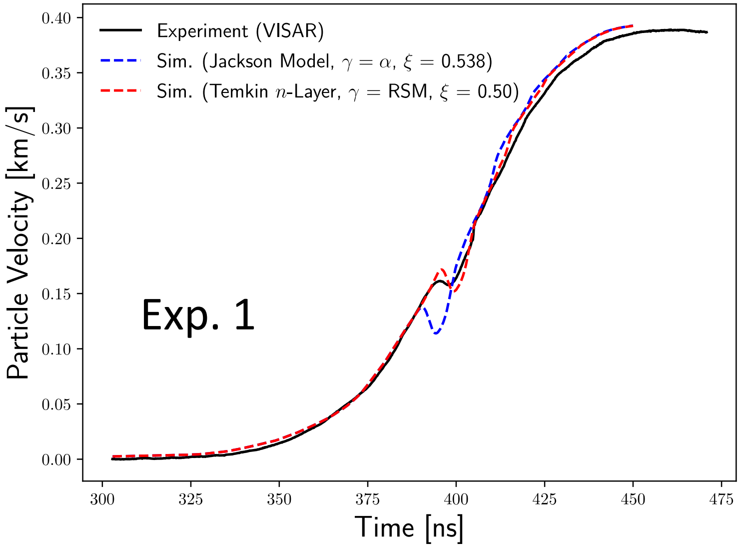


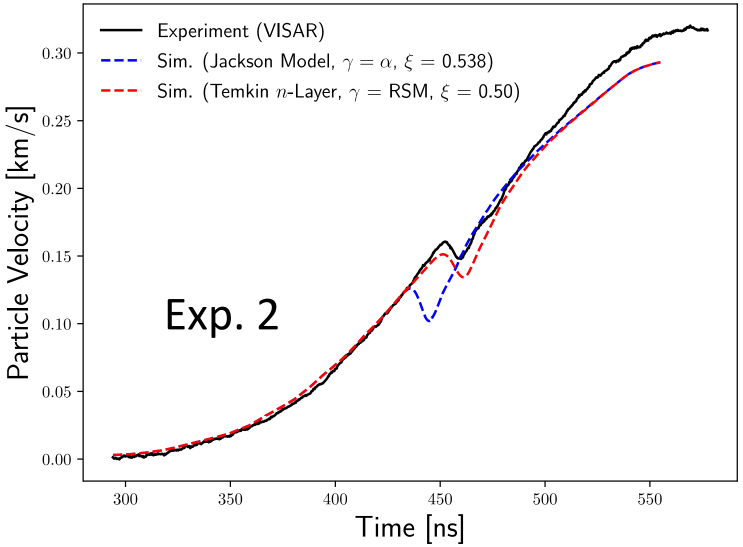
(with small amount of empirical refinement)

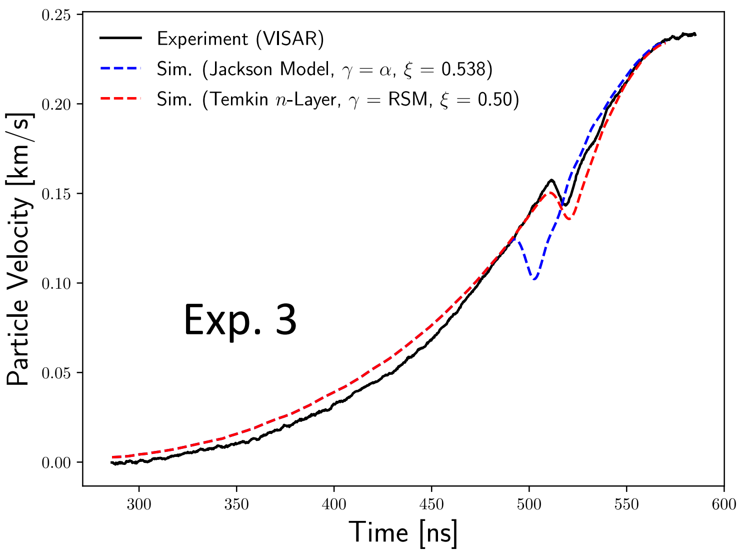
Mass	Momentum	Energy
$\frac{D\rho}{Dt} = -\rho\nabla \cdot u$	$\rho\frac{Du}{Dt} = -\nabla P(\phi)$	$\rho\frac{DE}{Dt} = -P(\phi)\nabla \cdot u$

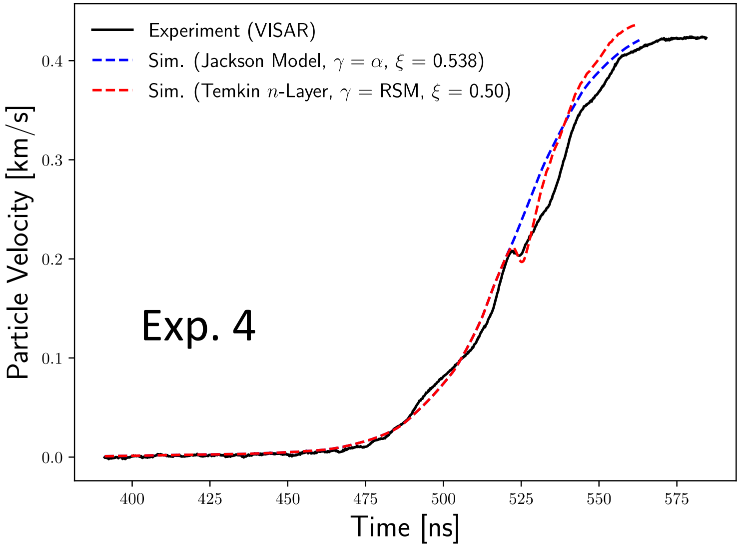
Simulations result in excellent agreement for Nissen and Dolan Experiments [1] (Magnetic Drive)

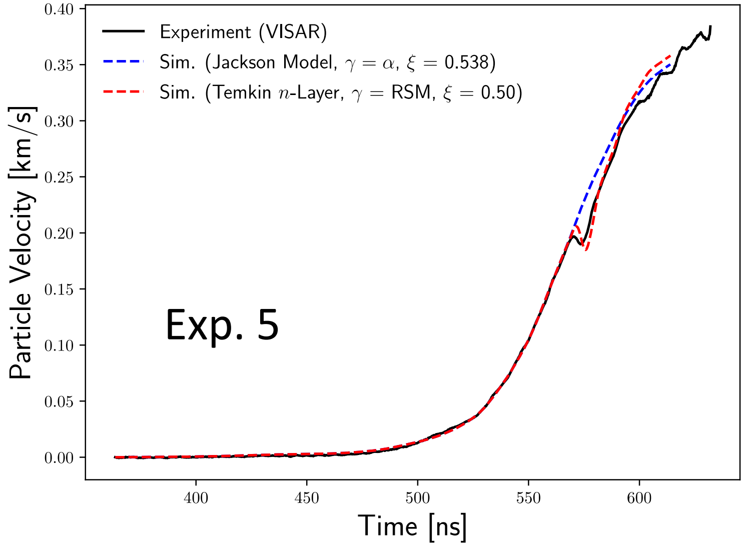


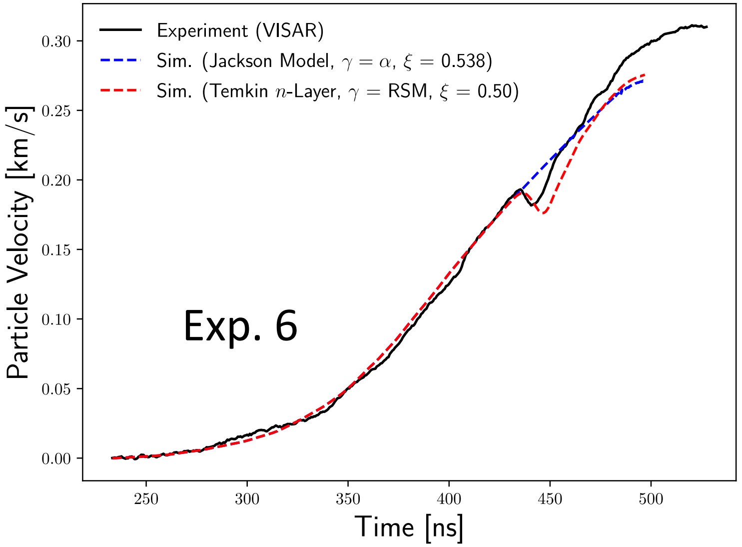




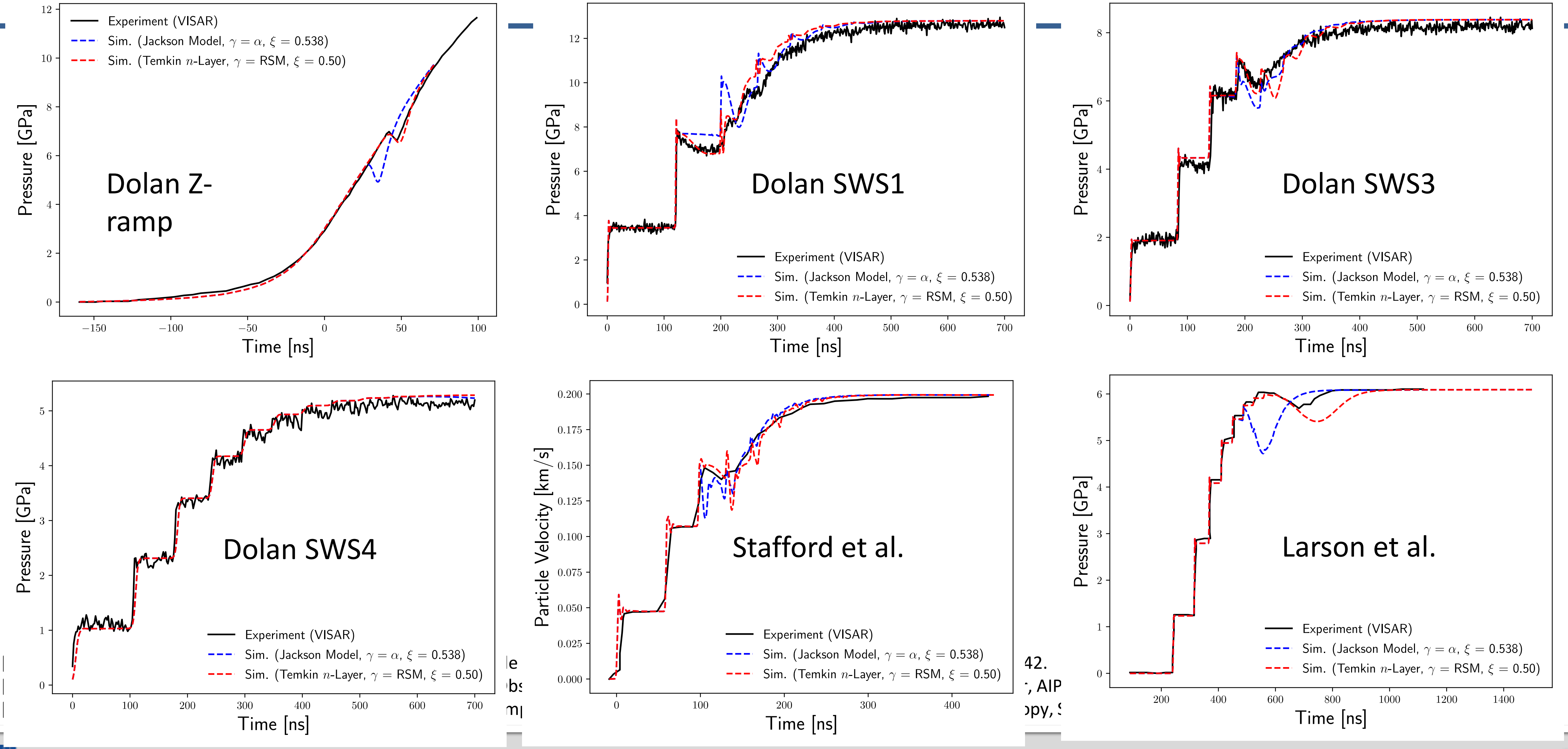








Simulations result in excellent agreement for the Dolan et al. [1], Stafford et al. [2], and Larson et al. [3] experiments



Conclusions

- Our kinetics models can directly account for transient phase transition kinetics
- Also accounts for discrepancies in the phase transition timescales/transition pressure found in experiments
- Developed novel methodology to solve ramp-wave compression drive-pressure inverse problem for experiments with different drive mechanisms (e.g., magnetic drive, laser drive, does not require knowledge of drive-specific physics)
- Applied a multilayer interface model to better characterize solid—liquid interface of nucleating ice VII clusters
- Future Work: Molecular dynamics simulations will be needed to further characterize the interface and benchmark results of using the Temkin *n*-layer model
- This work has led to several current/future journal publications:
  - **(1) D. M. Sterbentz, P. C. Myint, J. P. Delplanque, J. L. Belof (2019), "Numerical modeling of solid-cluster evolution applied to the nanosecond solidification of water near the metastable limit," The Journal of Chemical Physics, 151(16), 164501.**
  - **(2) D. M. Sterbentz, J. R. Gambino, P. C. Myint, J. P. Delplanque, H. K. Springer, M.C. Marshall, J. L. Belof (2020), "Drive-pressure optimization in ramp-wave compression experiments through differential evolution," Journal of Applied Physics 128, 195903.**
  - **(3) D. M. Sterbentz, P. C. Myint, J. P. Delplanque, J. L. Belof (2021), "Applying the Temkin *n*-layer model of the solid—liquid interface to the rapid solidification of water under dynamic compression," (in preparation for publication).**

Acknowledgments

University of California, Davis: Jean-Pierre Delplanque

Lawrence Livermore National Laboratory: Philip C. Myint, Jonathan L. Belof

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Lawrence Livermore National Laboratory