Exploration of Approaches to Shock-wave Simulation

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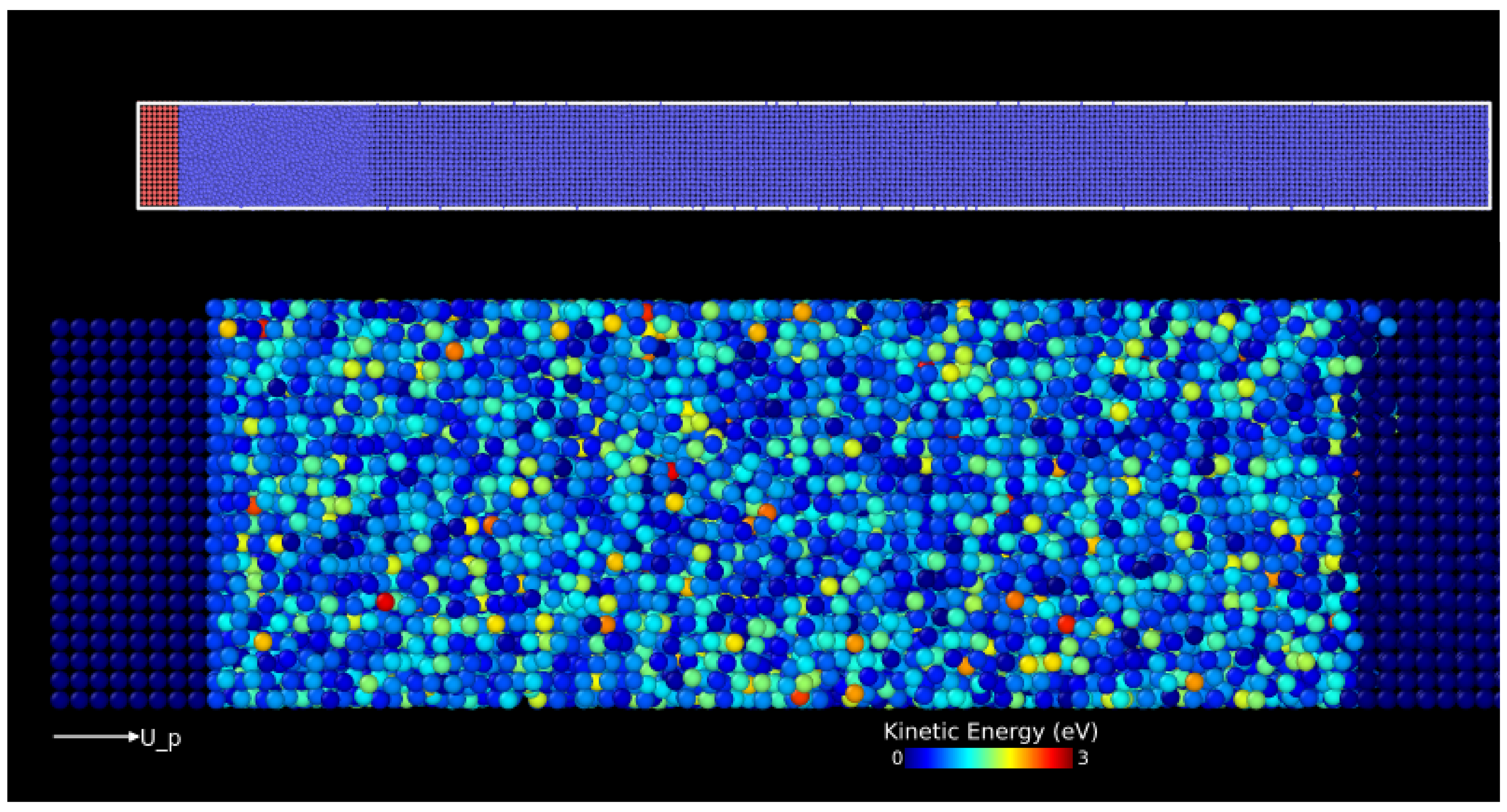
Why shock-waves?

- Shock-waves are everywhere: from breaking glass to meteorite impacts.
- Shock-waves primary method of exploring extreme pressures.
- Understanding how shock-waves affect materials, structure and properties, is vital for developing materials or new structures.

What are shock-waves?

- Shock-waves are defined by a wavefront moving through the material at a velocity greater than the speed of sound in the material.
- They are characterised by a rapid wave of elastic deformation followed or overtaken by a wave of plastic deformation.
- This plastic deformation results in defects and even crystal structure reordering.
- Shock-waves create a diverse mixture of states and highly disordered structures.



Snapshot of an NEMD shock-wave.

- The area just behind the shock front is the part in which we are most interested as it is here that the system is at its extreme.

Importance of Study

- Experimental high-pressure condensed matter physics use shock-waves extensively
- In order to corroborate this need accurate simulation techniques.
- Larger systems become too expensive to simulate accurately.
- Often shock-waves are simulated using empirical potentials.
- Empirical potentials fitted to stable systems.

Computational Challenges

- Systems for simulating shock-waves must be large enough for shock to have time to move through.
- Shock-wave simulations require very short time-steps to prevent the system destabilising:
  - This means more time-steps are needed to pass the same real-time.
- Want whole Hugoniot, cover range of impact spaces need multiple runs.
- Infeasible to run DFT NEMD!

Possible Salvation

- Maillet and Bernard [2] developed integrator to force system into shocked state.
- Uses Nosé-Hoover like integrator to control temperature and sometimes pressure to shocked state-point.

$$\dot{\mathbf{p}}_i = \mathbf{F}_i - \nu\chi\mathbf{p}_i; \quad \dot{\chi} = \frac{\nu}{C}(E(t) - E_H(t))$$

$$E_H(t) = E(t_0) + \tfrac{1}{2}(P(t) + P(t_0))(V(t_0) - V(t))$$

- Requires good coupling ν which is difficult to know initially.
- Initial transient states.
- Need scaling parameter for system.

Methods

The following have been implemented in the CASTEP code [1].

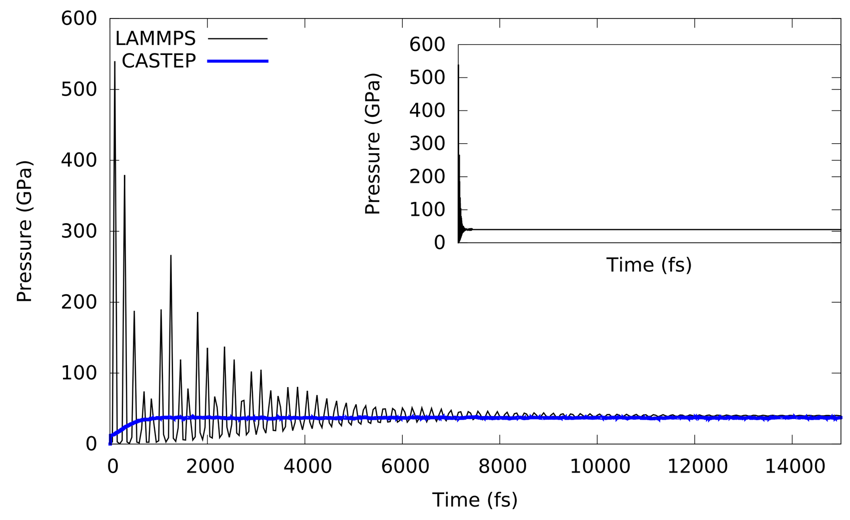
We have taken the idea of the Hugoniostat and extended this in a variety of ways:

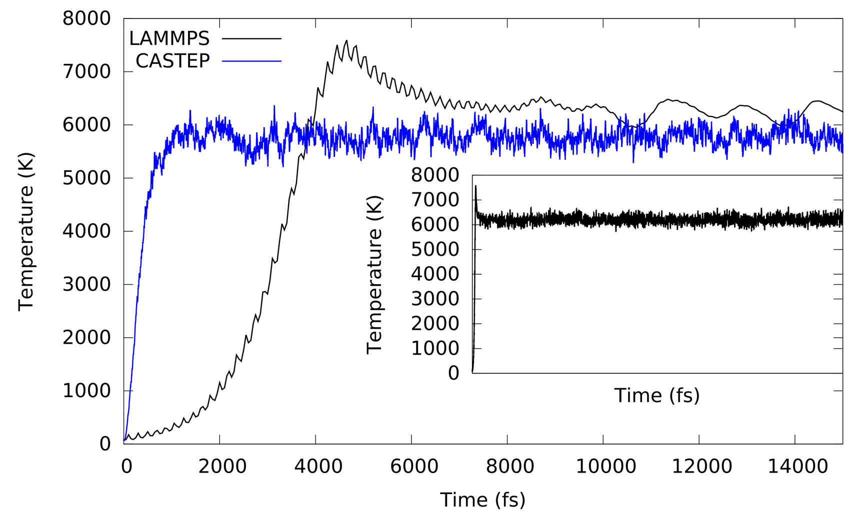
- Reformulated as a Langevin integrator (ensuring ergodicity)

$$\dot{\mathbf{p}}_i = \mathbf{F}_i - \gamma\mathbf{p}_i + \sqrt{\frac{2m_i k_B T\gamma}{\Delta t}}N(0,1)$$

$$\dot{T} = \frac{-\Delta t T_0}{\nu C}(E(t) - E_H(t))$$

where γ is damping, ν is coupling, C is scaling

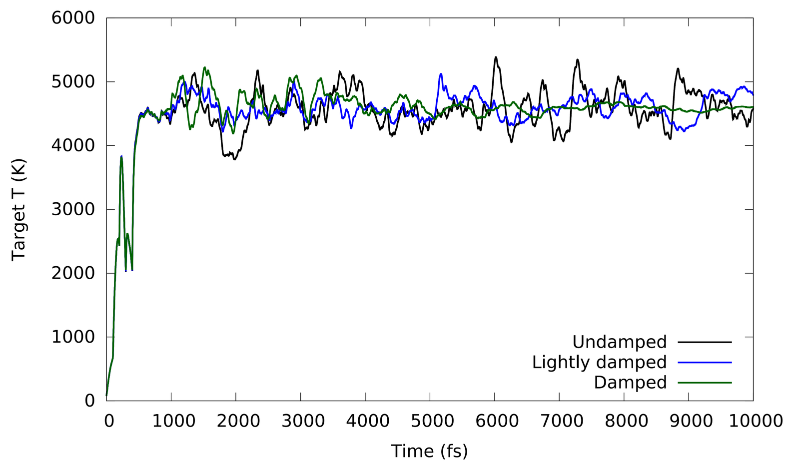


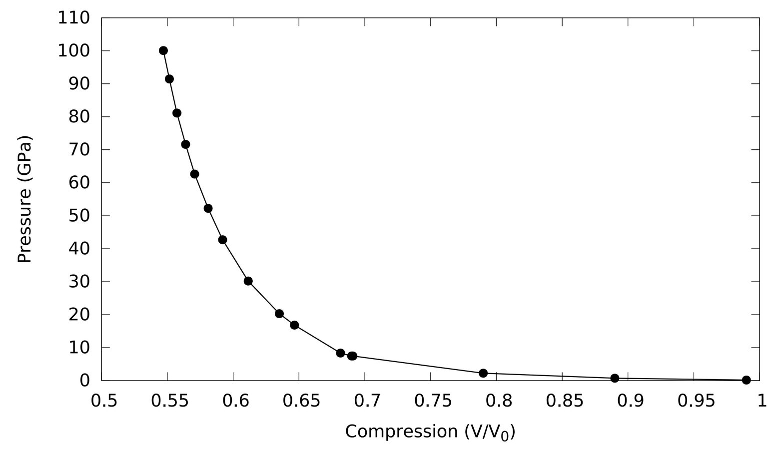


- Applied a damping mechanism to the coupling.

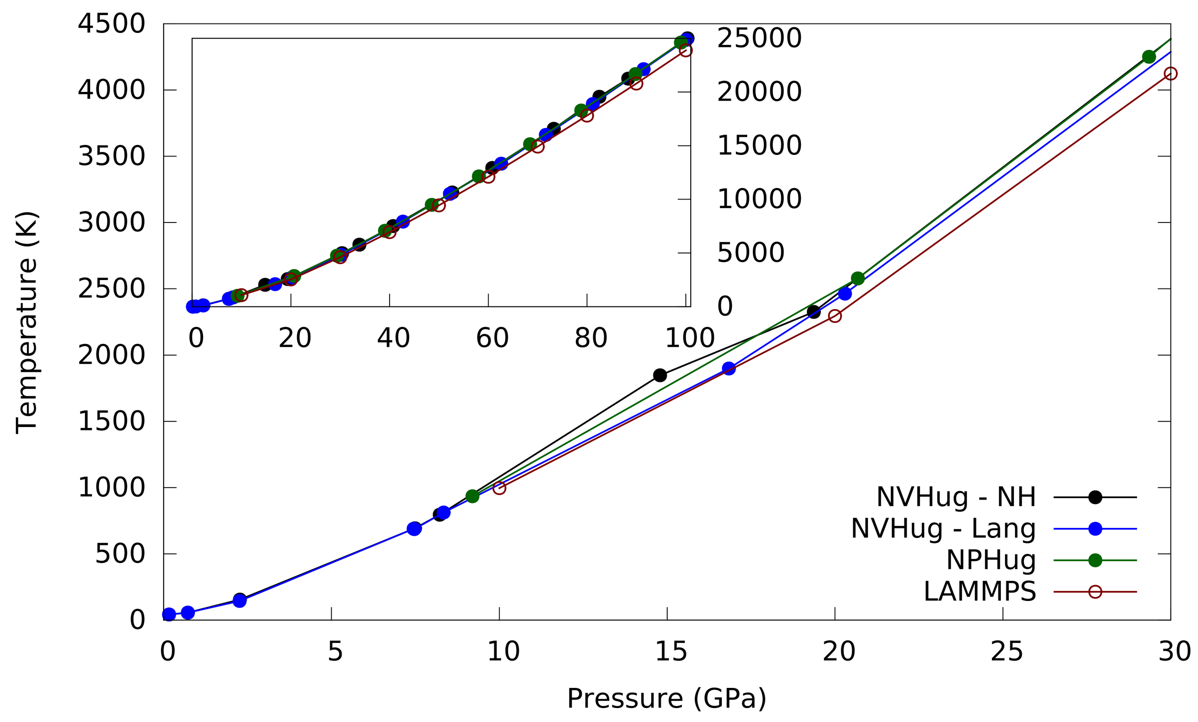
$$\text{if } \chi\dot{\chi} < 0: \qquad \nu = A\nu$$

where A is some scaling constant which is < 1





- Applied a predictor algorithm to the method allowing a single run to use old parameters:
  - Means we can use more efficient, less convenient algorithm to scan pressure space.
  - Allows predicted coupling and reuse of old state.
  - Can detect discontinuities in the Hugoniot.



Future Work

- Find reliable material dependent scaling factor.
- Apply method to DFT simulation.
- Extend method to automate more fully.
- Provide more methods for sampling material properties.

References

[1] "First principles methods using CASTEP", Zeitschrift fuer Kristallographie 220(5-6) pp. 567-570 (2005) S. J. Clark, M. D. Segall, C. J. Pickard, P. J. Hasnip, M. J. Probert, K. Refson, M. C. Payne

[2] Jean-Bernard Maillet and Stéphane Bernard. Uniaxial hugoniostat: Method and applications. In *Shock Compression of Condensed Matter*. American Institute of Physics, *2001*.