U.S. ARMY RESEARCH, DEVELOPMENT AND ENGINEERING COMMAND

Accelerating Scale Bridging via Surrogate Modeling

Jaroslaw Knap[1], Ting Wang[1], Kenneth W. Leiter[1] and Petr Plechac[2]

[1]U.S. Army Research Laboratory, [2]University of Delaware

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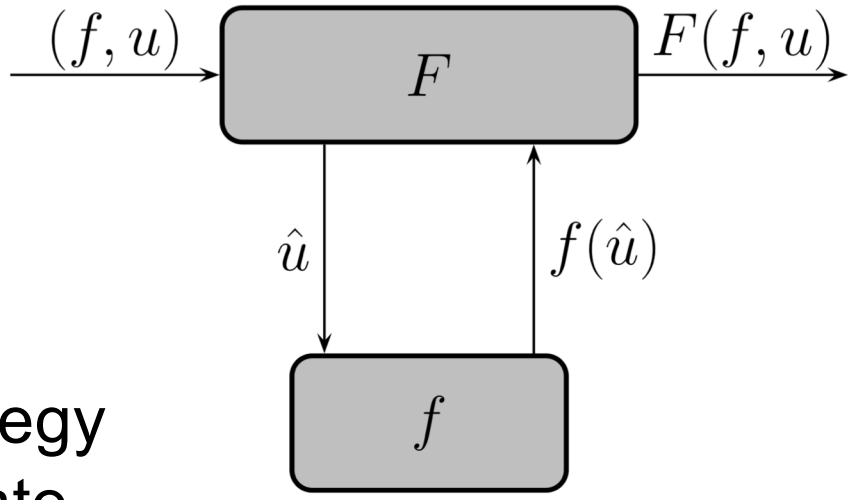
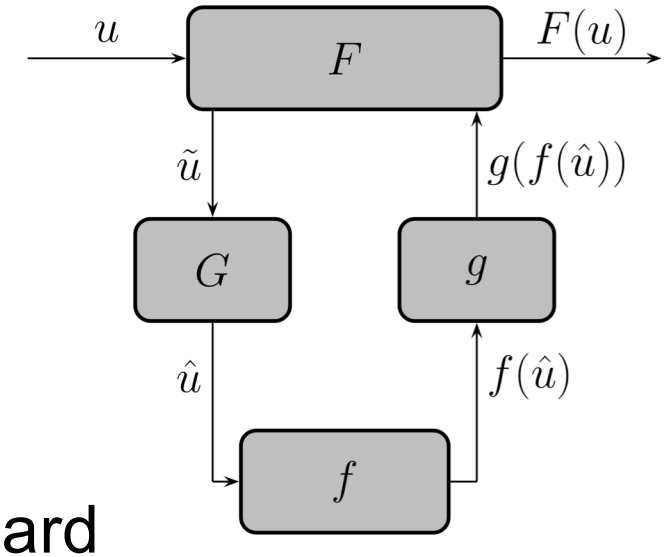
MULTISCALE MODELING

- Multiscale modeling: a systematic approach to development of high-fidelity material models
- Combine physics associated with relevant scales
- Two-scale model:
  - F acquires missing data from f
  - Communicate $\hat{u}$
  - Assimilate $f(\hat{u})$
- Divide-and-conquer strategy allows to easily incorporate disparate physics



MULTISCALE MODELING

- Computation fundamental in multiscale modeling
- Many high-fidelity computational at-scale models are available
- Scale bridging
  - Communicate $\tilde{u}$
  - Evaluate $f(\hat{u})$
  - Carry out data estimation $g\big(f(\hat{u})\big)$
  - Communicate $g\big(f(\hat{u})\big)$
- Scale bridging essential, but can be hard and computationally challenging

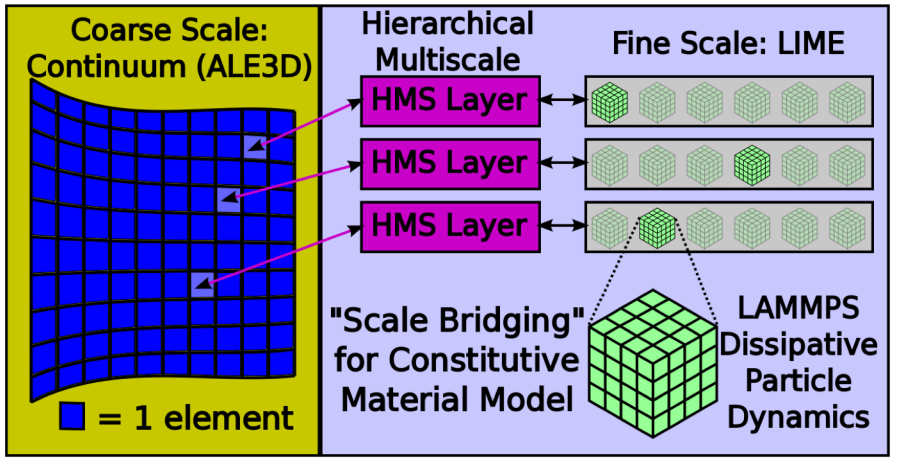


TWO-SCALE MODEL OF RDX

- Goal: develop high-fidelity model of RDX
- Difficulty: incorporate effects of chemical decomposition
- Two scale model
  - Upper-scale model: FEM
    - Equation of state obtained from the lower-scale model

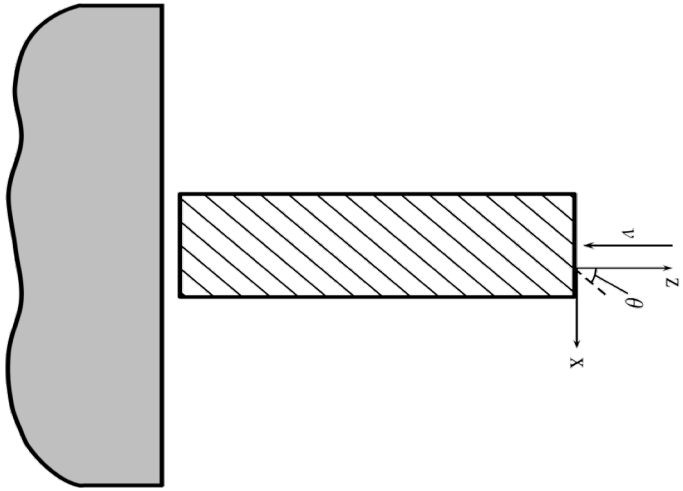
$$(p, T) = f(\rho, e)$$

    - J2-plasticity strength model
  - Lower-scale model: DPD-E LAMMPS
    - RDX single crystal with no defects
    - No chemistry

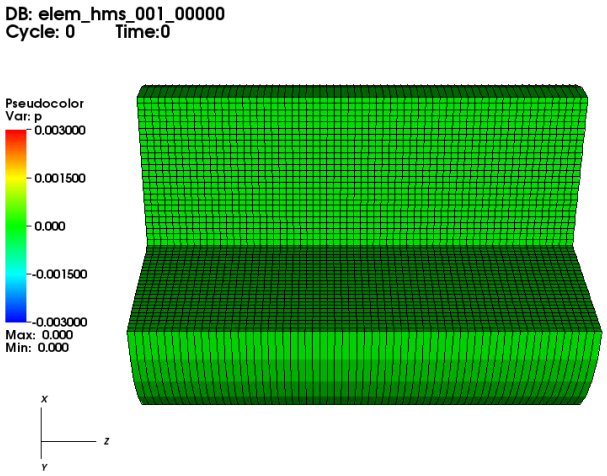


TWO-SCALE MODEL OF RDX

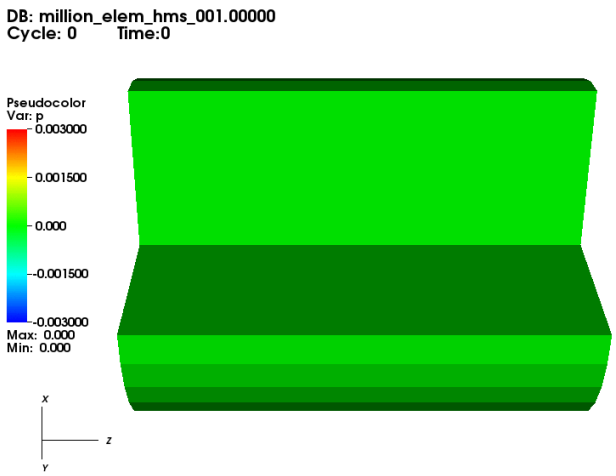
- Simulation Details
  - Cylinder of RDX impacting rigid anvil at 200 m/s
  - 2D (axisymmetric) model
  - 1,600 elements



Left: 1600 elements



Right: 1 million elements



pressure (Mbar)

TWO-SCALE MODEL OF RDX

- 1 million element simulations computationally intractable with simple on-the-fly approach
  - Approximately 25 billion cpu hours to complete
  - ARL's biggest computer offers the total of 868 million cpu hours in a year
- Lower-scale models bound to get even more expensive
  - With inclusion of relatively simple chemistry the cost of our DPD RDX model increases 4 fold
- Significantly reduce the cost of lower-scale models by surrogate modeling
- Surrogate model is an approximation of a model, constructed from direct observations of the model