CoEVP (Embedded ViscoPlasticity) Scale-bridging Proxy App

git@github.com:exmatex/CoEVP.git

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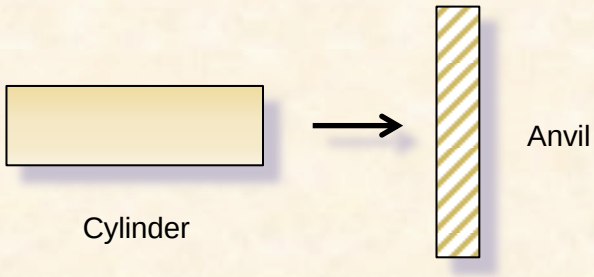
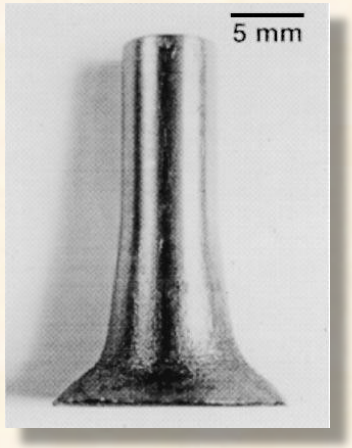
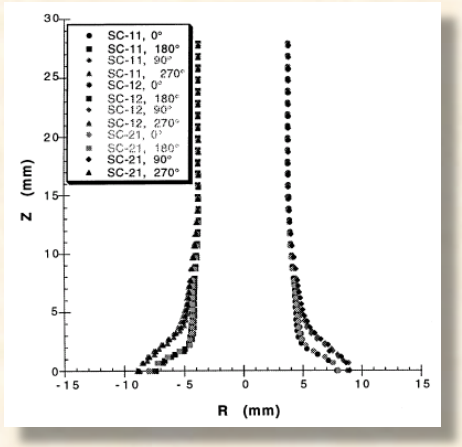
CoEVP uses scale-bridging to solve a Taylor cylinder impact test problem

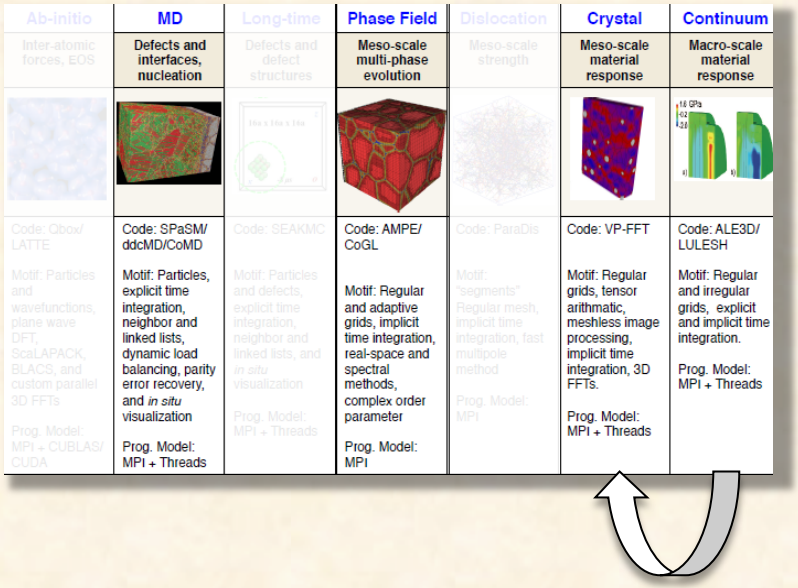


- A tantalum cylinder is fired into a stationary wall.
- The fine-scale details of the material microstructure determine the coarse-scale deformation at the impact surface





Source: P. J. Maudlin, J. F. Bingert, J. W. House, S. R. Chen, "On the modeling of the Taylor cylinder impact test for orthotropic textured materials: experiments and simulations", Inter. J. Plasticity 15 (1999), pp. 139-166.



CoEVP adds strength to LULESH which provides the coarse-scale model

Lagrangian coordinates:

$$\mathbf{x} \equiv \mathbf{x}(t), \qquad \mathbf{x}(0) = \mathbf{x}_0,$$
$$\mathbf{v} \equiv \dot{\mathbf{x}}(t), \qquad \mathbf{v}(0) = \mathbf{v}_0,$$

Momentum:

$$\rho\dot{\mathbf{v}} = \boxed{\nabla \cdot \boldsymbol{\sigma}} + \rho\mathbf{f}$$

Energy:

$$\rho_0\dot{e} = \boxed{\eta\boldsymbol{\sigma}' : \mathbf{L}} - (p+q)\,\dot{\eta}$$

where

$$\boldsymbol{\sigma}' \equiv \boldsymbol{\sigma} + \boxed{(p} + \boxed{q)}\mathbf{I},$$
$$\mathbf{L} \equiv \frac{1}{2}\left(\nabla\mathbf{v} + (\nabla\mathbf{v})^T\right),$$
$$p \equiv -\frac{1}{3}\mathrm{tr}(\boldsymbol{\sigma}) - q$$

$\mathbf{x}$	position
$\mathbf{v}$	velocity
$\rho = \rho_0\eta^{-1}$	density
ρ_0	reference density
η	relative volume
$\boxed{\boldsymbol{\sigma}}$	Cauchy stress
$\boldsymbol{\sigma}'$	deviatoric Cauchy stress
$\mathbf{f}$	specific body force
e	specific internal energy
$\boxed{p}$	pressure
$\boxed{q}$	bulk viscosity
$\mathbf{L}$	velocity gradient

Constitutive model evaluation requires the integration of an intermediate system involving multiple fine-scale model evaluations

Stress tensor is obtained from an elasticity model:

$$\bar{\sigma} = -(p+q)\,\mathbf{I} + J^{-1}\frac{2G}{a}\bar{\mathbf{V}}'$$

that depends upon an evolving strain tensor deviator $\bar{\mathbf{V}}'$ obtained from the solution of a kinematic system:

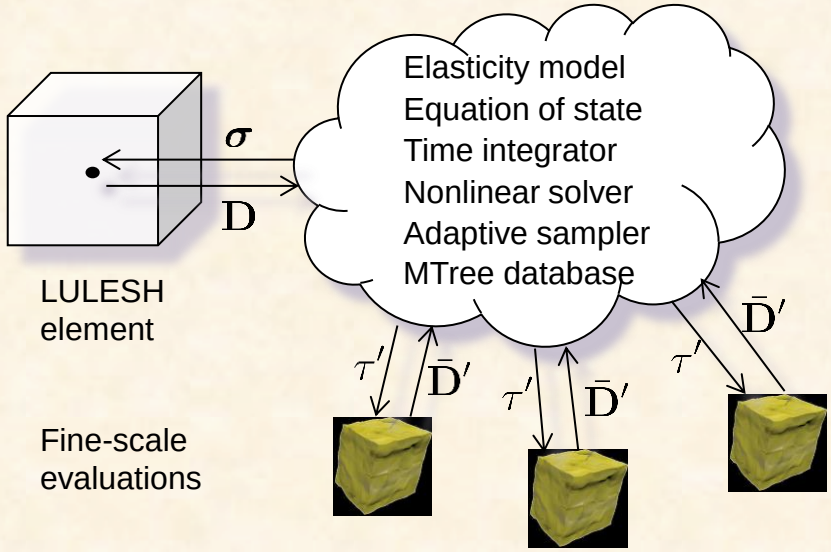
from coarse-scale model

from fine-scale model

$$\frac{1}{a}\dot{\bar{\mathbf{V}}}' = \mathbf{R}^{\mathrm{T}}\cdot\mathbf{D}'\cdot\mathbf{R} - \bar{\mathbf{D}}',$$

$$\dot{J} = J\mathrm{tr}(\mathbf{D}),$$

$$\begin{aligned}\dot{\mathbf{R}}\cdot\mathbf{R}^{\mathrm{T}} &= \mathbf{W}^{\mathrm{R}} \\ &= \mathbf{W} - \mathbf{R}\cdot\bar{\mathbf{W}}\cdot\mathbf{R}^{\mathrm{T}} \\ &\quad - \frac{1}{a}\mathbf{R}\cdot\left[\bar{\mathbf{V}}'\cdot\left(\bar{\mathbf{D}}' + \frac{1}{2a}\dot{\bar{\mathbf{V}}}'\right) - \left(\bar{\mathbf{D}}' + \frac{1}{2a}\dot{\bar{\mathbf{V}}}'\right)\cdot\bar{\mathbf{V}}'\right]\cdot\mathbf{R}^{\mathrm{T}}\end{aligned}$$



Heterogeneous computing model and approach closely follows LLNL Coop project:

N. R. Barton et al., “Embedded polycrystal plasticity and adaptive sampling”, International Journal of Plasticity 24 (2008), pp. 242-266.

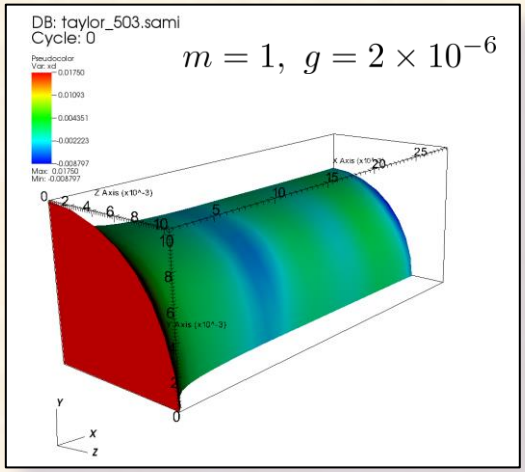
Current approach: Use Taylor model parameters to vary fine-scale model evaluation workflow

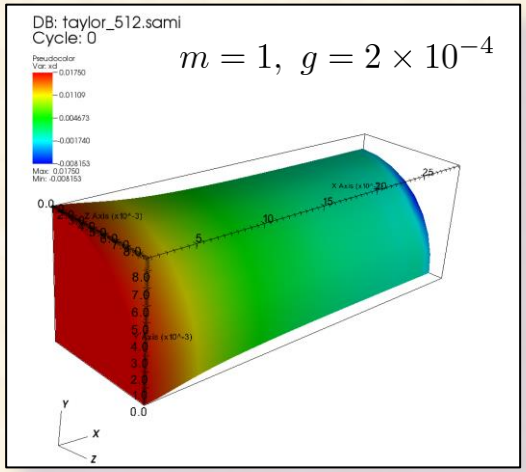
Workflow:

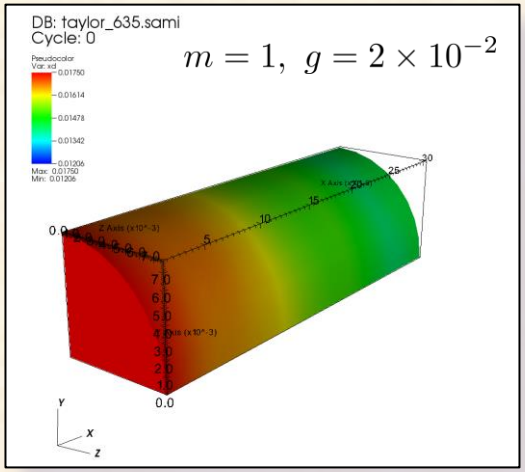
- Spatial and temporal distribution of the fine-scale model queries
- Cost of the fine-scale queries
  - Fine-scale model evaluation
  - Database look-up (interpolation)

$$\bar{\mathbf{D}}' = D_0 \frac{\bar{\tau}'}{||\bar{\tau}'||} \left(\frac{||\bar{\tau}'||}{g} \right)^m$$

m	Sensitivity
g	Hardness
D_0	Scaling factor







Integration of the kinematic system with a Taylor fine-scale model

Constitutive model provides

$$\bar{\sigma} = -(p+q)\,\mathbf{I} + \bar{\sigma}'$$

Assume elasticity model

$$\bar{\boldsymbol{\tau}}' = 2G\bar{\mathbf{E}}' \approx \frac{2G}{a}\bar{\mathbf{V}}'$$

where

$$\bar{\sigma}' = J^{-1}\bar{\boldsymbol{\tau}}'$$

$$a = J^{1/3}$$

$$\mathbf{E} = \ln(\mathbf{V})$$

Stretch tensor rate equation

$$\frac{1}{a}\dot{\bar{\mathbf{V}}}' = \mathbf{R}^{\mathrm{T}}\cdot\mathbf{D}'\cdot\mathbf{R} - \bar{\mathbf{D}}',$$

$$= \mathbf{R}^{\mathrm{T}}\cdot\mathbf{D}'\cdot\mathbf{R} - D_0\frac{\bar{\boldsymbol{\tau}}'}{||\bar{\boldsymbol{\tau}}'||}\left(\frac{||\bar{\boldsymbol{\tau}}'||}{g}\right)^m$$

If $m = 1$

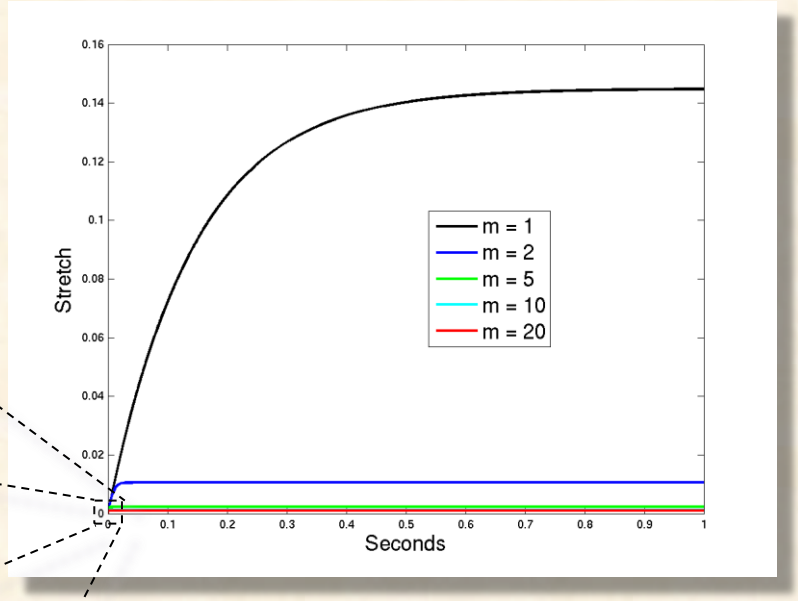
$$\frac{1}{a}\dot{\bar{\mathbf{V}}}' = \mathbf{R}^{\mathrm{T}}\cdot\mathbf{D}'\cdot\mathbf{R} - \frac{b}{a}\bar{\mathbf{V}}'$$

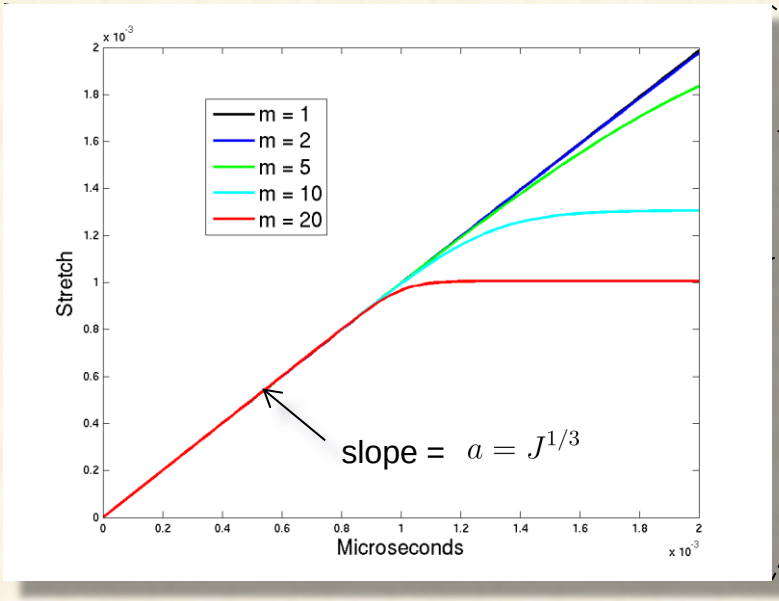
where $b \equiv \dfrac{2D_0G}{g}$

$$\bar{\mathbf{V}}'(t) = \frac{a}{b}\mathbf{R}^{\mathrm{T}}\cdot\mathbf{D}'\cdot\mathbf{R} + e^{-bt}\left[\bar{\mathbf{V}}'(0) - \frac{a}{b}\mathbf{R}^{\mathrm{T}}\cdot\mathbf{D}\cdot\mathbf{R}\right]$$

Taylor model parameters determine the viscoplastic transition

- m determines the transition sharpness
- G/g determines the location
- D_0 plays a decreasing role as m increases





Tantalum cylinder test problem:

$$D_0 = 1 \times 10^{-2}\ \mu\text{s}^{-1}$$

$$G = 6.9 \times 10^{-1}\ \text{Mbar}$$

$$g = 2 \times 10^{-3}\ \text{Mbar}$$

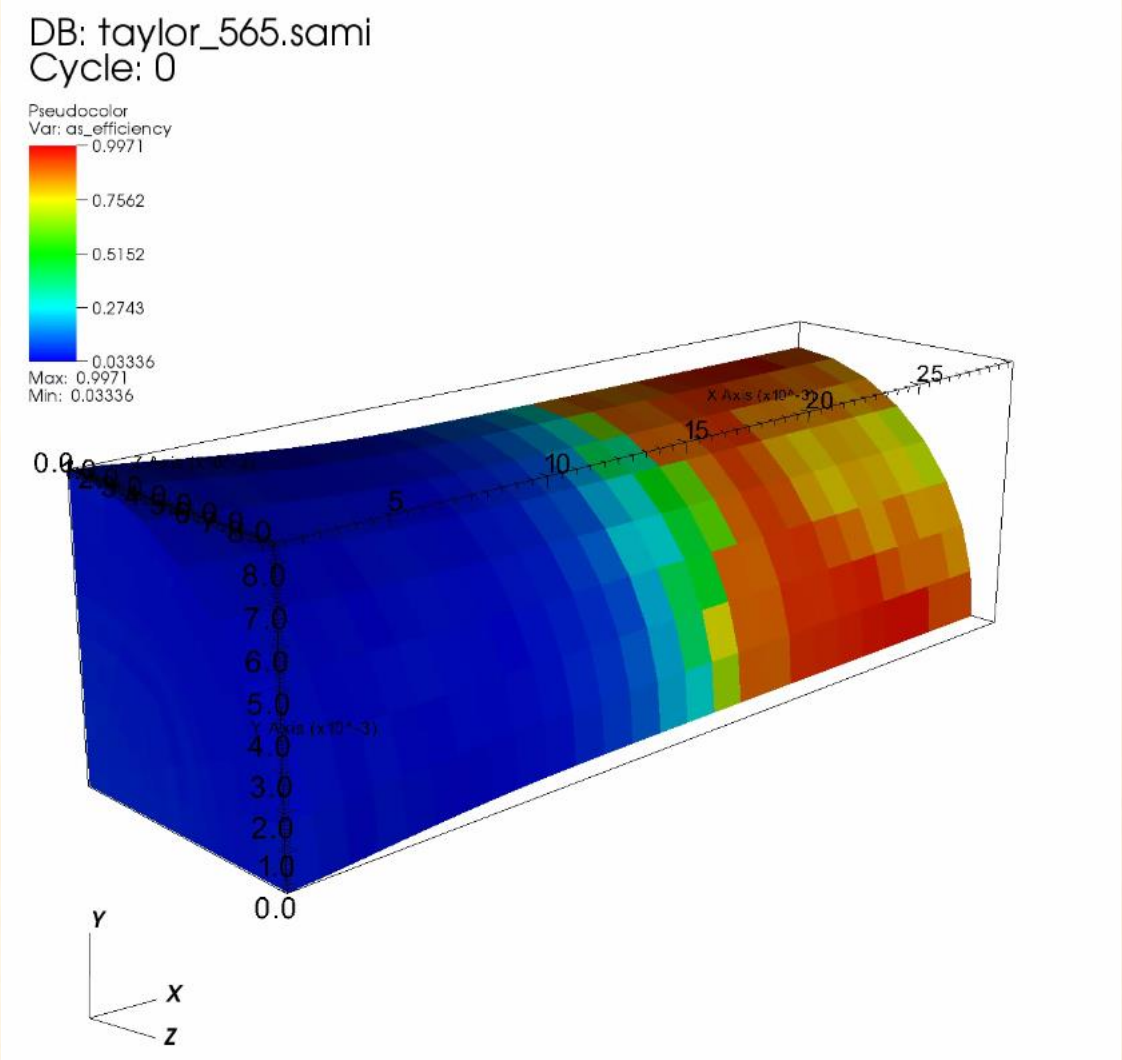
LULESH stable $\Delta t \approx 1.5 \times 10^{-4}\ \mu\text{s}$

Nonlinear solver requires increasing globalization as the sensitivity parameter m increases

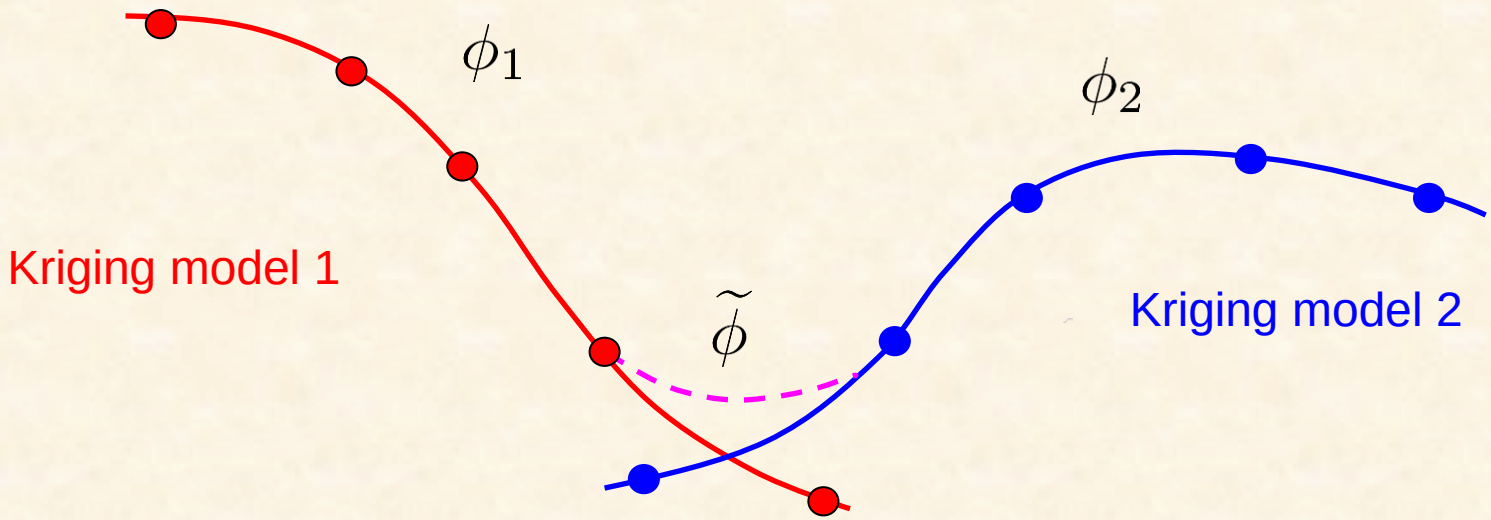
m	Newton solver performance without globalization
1	1 iteration
2	few iterations
≥4	more iterations and loss of quadratic convergence

- Tantalum model requires m = 20
- Remedies
  - Monitor the number of Newton solves and reduce the coarse scale time step if a threshold is exceeded
  - Add a globalization strategy to the Newton solve
    - » Backtracking
    - » Trust region

CoEVP adaptive sampling efficiency plots provide some workflow information



The “C0 problem”

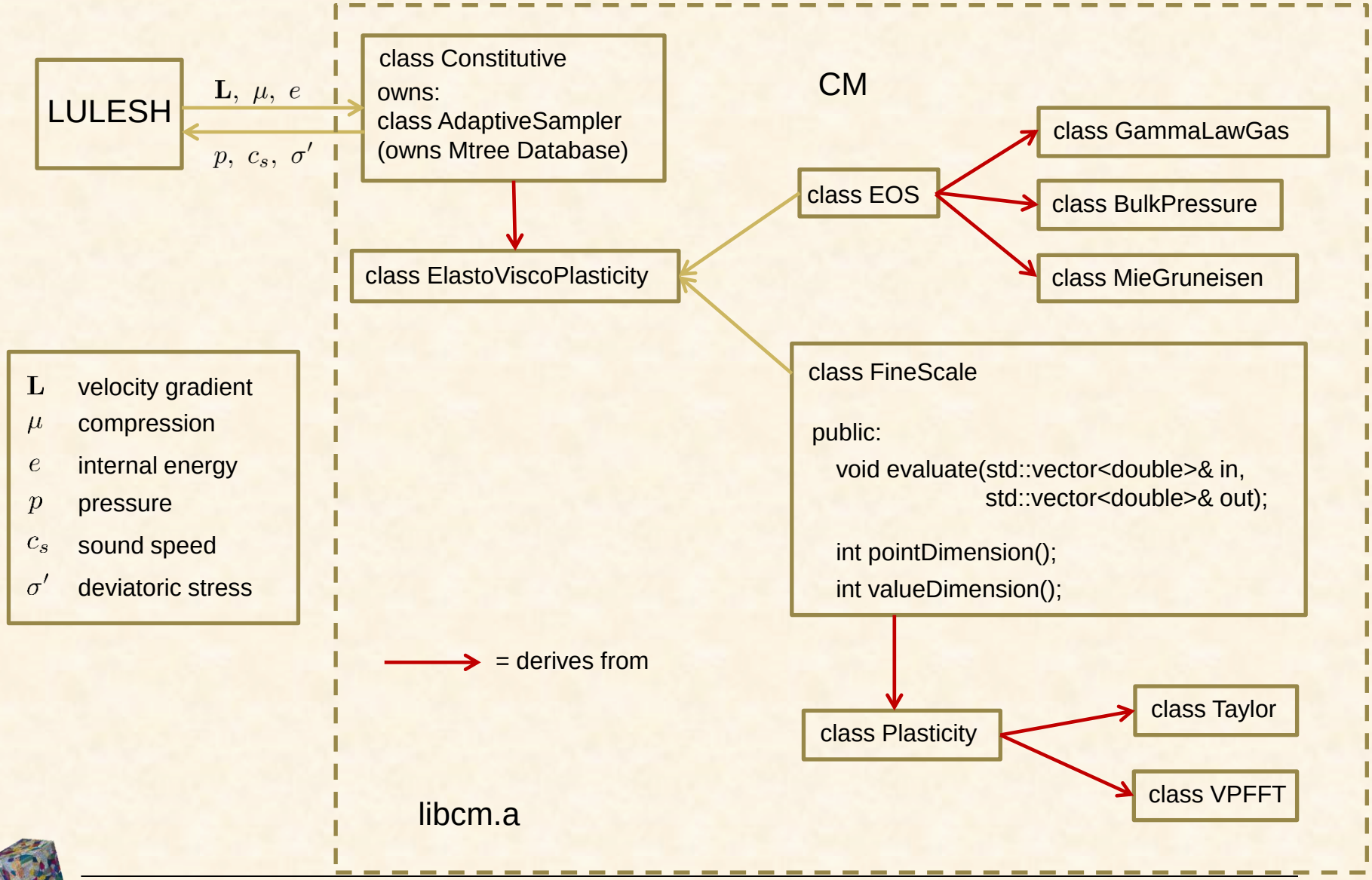


$$\widetilde{\phi} = w(e_1)\phi_1 + w(e_2)\phi_2$$

Kriging interpolation error estimators

$$\lim_{e \to \tau} w(e) = 0$$

CoEVP is ready to begin implementation of the heterogeneous computing model



$\mathbf{L}$	velocity gradient
μ	compression
e	internal energy
p	pressure
c_s	sound speed
σ'	deviatoric stress