A Specification for an Elastoviscoplasticity Scale-bridging Proxy App for ExMatEx

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1 Introduction

The purpose of this document is to specify an elastoviscoplasticity proxy application that employs scale bridging to couple a Lagrangian finite element model of the coarse "engineering" scale with an embedded viscoplasticity fine scale model of high strain rate material constitutive properties. The approach closely follows that of [3] in which a viscoplasticity model was embedded in ALE3D using an adaptive sampling approach. Due to the size and complexity of ALE3D, as well as restrictions on its distribution, we seek a simplification of this earlier work in which the currently available LULESH and VPFFT proxy apps provide the coarse- and fine-scale model implementations, respectively. This will better enable vendors and other researchers to investigate the implications and requirements of scale-bridging applications on exascale platforms.

2 Coarse-scale model

Lagrangian model

The macroscopic motion of the material system is described by a Lagrangian model of the evolution of position and velocity coordinates, $\mathbf{x}$ and $\mathbf{v}$,

$$\mathbf{x} \equiv \mathbf{x}(t), \qquad \mathbf{x}(0) = \mathbf{x}_0, \tag{1}$$

$$\mathbf{v} \equiv \dot{\mathbf{x}}(t), \qquad \mathbf{v}(0) = \mathbf{v}_0, \tag{2}$$

coupled with a momentum equation

$$\rho\dot{\mathbf{v}} = \nabla \cdot \boldsymbol{\sigma} + \rho\mathbf{f}, \tag{3}$$

where $\rho = \rho_0\eta^{-1}$ is the density, ρ_0 is a reference density, η is the relative volume, $\boldsymbol{\sigma}$ is the Cauchy stress tensor and $\mathbf{f}$ is a body force density (*e.g.*, gravity). The specific internal energy e is evolved as

$$\rho_0\dot{e} = \eta\boldsymbol{\sigma}'{:}\mathbf{L} - (p+q)\,\dot{\eta}. \tag{4}$$

Here, $q = q(\mathbf{v})$ is the bulk viscosity, and the deviatoric stress, velocity gradient and pressure are given by

$$\boldsymbol{\sigma}' \equiv \boldsymbol{\sigma} + (p+q)\,\mathbf{I}, \tag{5}$$

$$\mathbf{L} \equiv \frac{1}{2}\left(\nabla\mathbf{v} + (\nabla\mathbf{v})^T\right), \tag{6}$$

$$p \equiv -\frac{1}{3}\mathrm{tr}(\boldsymbol{\sigma}) - q, \tag{7}$$

$$\boldsymbol{\sigma}'{:}\mathbf{L} \equiv \mathrm{tr}\left(\boldsymbol{\sigma}' \cdot \mathbf{L}^T\right), \tag{8}$$

respectively. To close the system, a constitutive model is required to specify $\boldsymbol{\sigma}$.

The system of equations (1)-(8) is the same as that solved by both ALE3D and LULESH, although, for simplification purposes in its role as a proxy app, LULESH includes only the volumetric stress component (*i.e.*, $\boldsymbol{\sigma}' = 0$), and the pressure is given by an ideal gas law $p = (\gamma - 1)\rho e$.

Discretization

A finite element method is used to discretize (1)-(8). Letting Ω denote the spatial domain, a variational formulation of (3) is obtained by integrating it against a suitable space of test functions w, using integration by parts on the divergence term:

$$\int_\Omega \rho\dot{\mathbf{v}} dw\Omega + \int_\Omega \boldsymbol{\sigma}\cdot\nabla w d\Omega - \int_\Gamma \mathbf{n}\cdot\boldsymbol{\sigma} d\Gamma = \int_\Omega \rho\mathbf{f} w d\Omega, \qquad \forall w, \tag{9}$$

where $\Gamma \equiv \partial\Omega$ is the boundary of Ω and $\mathbf{n}$ is its outward-pointed unit normal. The spatial discretization results from limiting the position coordinate $\mathbf{x}$ (and therefore also $\mathbf{v}$) to a finite-dimensional subspace, as well as limiting the space of test functions to the same, or possibly different, finite-dimensional space. Numerical quadrature is then used to compute the integrals in the discrete variational form. Consequently, we require evaluations of $\boldsymbol{\sigma}$ at the corresponding quadrature points.

3 Strength model

Strain measure

Specification of the constitutive model yielding $\boldsymbol{\sigma}$ requires the introduction some measure of material strain together with a prescription for its evolution over a coarse-scale time step. As described in [3], the coarse-scale model couples to the fine-scale viscoplasticity model through a factorization of the material deformation gradient

$$\mathbf{F} = \mathbf{V}\cdot\mathbf{R}\cdot\mathbf{F}^p \tag{10}$$

into a symmetric, thermo-elastic stretch tensor $\mathbf{V}$, a rotation $\mathbf{R}$ between the fine- and coarse-scale reference frames, and a plastic deformation gradient $\mathbf{F}^p$. Since, by the chain rule,

$$\dot{\mathbf{F}} = \mathbf{L}\cdot\mathbf{F}, \tag{11}$$

the coarse-scale velocity gradient (6) may be evaluated using (10) as

$$\begin{aligned}\mathbf{L} &= \dot{\mathbf{F}} \cdot \mathbf{F}^{-1} \\ &= \dot{\mathbf{V}} \cdot \mathbf{V}^{-1} + \mathbf{V} \cdot \left(\dot{\mathbf{R}} \cdot \mathbf{R}^{\mathrm{T}} + \mathbf{R} \cdot \bar{\mathbf{L}} \cdot \mathbf{R}^{\mathrm{T}} \right) \cdot \mathbf{V}^{-1},\end{aligned} \tag{12}$$

where the fine-scale velocity gradient is defined as

$$\bar{\mathbf{L}} = \dot{\mathbf{F}}^{p} \cdot (\mathbf{F}^{p})^{-1}. \tag{13}$$

The kinematic system (12) therefore describes the evolution of $\mathbf{V}$ and $\mathbf{R}$ in terms of $\mathbf{L}$ and $\bar{\mathbf{L}}$. The integration of this system, which involves evaluations of the fine-scale plasticity model to obtain $\bar{\mathbf{L}}$, is described in Section 4. Using the resulting $\mathbf{V}$, we compute the logarithmic thermo-elastic strain measure

$$\mathbf{E} = \ln(\mathbf{V}). \tag{14}$$

Elasticity model

Letting

$$J = \det(\mathbf{V}), \quad a = J^{1/3}, \tag{15}$$

the volumetric component of $\bar{\mathbf{E}} = \mathbf{R}^{\mathrm{T}} \cdot \mathbf{E} \cdot \mathbf{R}$ (i.e., $\mathbf{E}$ in the fine-scale frame) is given by

$$\operatorname{tr}\left(\bar{\mathbf{E}}\right) = \ln\left(J\right), \tag{16}$$

and the deviatoric component approximated by

$$\bar{\mathbf{E}}' \approx \frac{1}{a}\bar{\mathbf{V}}'. \tag{17}$$

A simple elasticity model yielding the Cauchy stress $\boldsymbol{\sigma} = \mathbf{R} \cdot \bar{\boldsymbol{\sigma}} \cdot \mathbf{R}^{\mathrm{T}}$ needed by the coarse-scale model is

$$\bar{\boldsymbol{\sigma}} = -\left(p + q\right)\mathbf{I} + J^{-1}\bar{\boldsymbol{\tau}}' \tag{18}$$

where, assuming a constant shear modulus G, the deviatoric component of the Kirchoff stress $\boldsymbol{\tau} = J\boldsymbol{\sigma}$ is given by

$$\bar{\boldsymbol{\tau}}' = 2G\bar{\mathbf{E}}' = \frac{2G}{a}\bar{\mathbf{V}}'. \tag{19}$$

Equation of state and bulk viscosity

We assume that the pressure p is evaluated from the bulk pressure formula described in [2]:

$$p = p(\mu, e) \equiv p_g(\mu) + \rho_0 \left(\Gamma_0 + \alpha\mu\right) e, \tag{20}$$

where, defining the compression measure $\mu = \eta - 1$,

$$p_g(\mu) = \begin{cases} \dfrac{K_0\mu\left[1 + \left(1 - \frac{1}{2}\Gamma_0\right)\mu - \frac{1}{2}\alpha\mu^2\right]}{\left[1 - \left(S - 1\right)\mu\right]^2}, & \mu < 0, \\ K_0\mu, & \mu \geq 0, \end{cases} \tag{21}$$

where K_0, α and S are parameters. The bulk viscosity q is of the same monotonically limited form as currently implemented in LULESH, namely.

$$q = c_q\rho\left(a\nabla \cdot \mathbf{v}\right)^2 - c_\ell\rho c_s a|\nabla \cdot \mathbf{v}|, \tag{22}$$

where c_q and c_ℓ are parameters.

4 Integration of the kinematic system

Reformulation

As described in [3], the integration of (12) is facilitated by a reformulation in terms of the symmetric and skew components of the fine- and coarse-scale velocity gradients

$$\mathbf{D} = \frac{1}{2}\left(\mathbf{L} + \mathbf{L}^{\mathrm{T}}\right), \quad \mathbf{W} = \frac{1}{2}\left(\mathbf{L} - \mathbf{L}^{\mathrm{T}}\right), \tag{23}$$

$$\bar{\mathbf{D}} = \frac{1}{2}\left(\bar{\mathbf{L}} + \bar{\mathbf{L}}^{\mathrm{T}}\right), \quad \bar{\mathbf{W}} = \frac{1}{2}\left(\bar{\mathbf{L}} - \bar{\mathbf{L}}^{\mathrm{T}}\right). \tag{24}$$

The system is simplified by assuming that the deviatoric component of $\mathbf{V}$ is small

$$\mathbf{V} = \frac{1}{a}\left(\mathbf{I} - \epsilon^*\right), \tag{25}$$

and that plasticity does not affect the material volume

$$\mathrm{tr}(\bar{\mathbf{L}}) = \mathrm{tr}(\bar{\mathbf{D}}) = 0. \tag{26}$$

The resulting system (see [3]) is

$$\frac{1}{a}\dot{\bar{\mathbf{V}}}' = \mathbf{R}^{\mathrm{T}} \cdot \mathbf{D}' \cdot \mathbf{R} - \bar{\mathbf{D}}', \tag{27}$$

$$\dot{J} = J\mathrm{tr}(\mathbf{D}), \tag{28}$$

$$\begin{aligned} \dot{\mathbf{R}} \cdot \mathbf{R}^{\mathrm{T}} &= \mathbf{W}^{\mathrm{R}} \\ &= \mathbf{W} - \mathbf{R} \cdot \bar{\mathbf{W}} \cdot \mathbf{R}^{\mathrm{T}} \\ &\quad - \frac{1}{a}\mathbf{R} \cdot \left[\bar{\mathbf{V}}' \cdot \left(\bar{\mathbf{D}}' + \frac{1}{2a}\dot{\bar{\mathbf{V}}}'\right) - \left(\bar{\mathbf{D}}' + \frac{1}{2a}\dot{\bar{\mathbf{V}}}'\right) \cdot \bar{\mathbf{V}}'\right] \cdot \mathbf{R}^{\mathrm{T}}, \end{aligned} \tag{29}$$

where $\mathbf{A}'$ denotes the deviatoric part of a symmetric second order tensor $\mathbf{A}$. This is a system of nine equations in nine unknowns ($\mathrm{dof}(\bar{\mathbf{V}}') + \mathrm{dof}(J) + \mathrm{dof}(\mathbf{R}) = 5 + 1 + 3$). In addition to clarifying the dynamics described by the kinematic system (*e.g.*, (27) states that the deviatoric stretch component is determined by the difference between the coarse- and fine-scale strain rates), this reformulation also permits an important time scale issue to be addressed in the discrete integration.

Discrete time integration

In high strain rate applications, the right-hand side of (27) will be large, reflecting a fast time-scale relative to that of the coarse-scale model and necessitating an implicit time integration. Given its simple form, equation (28) can be integrated analytically, as can (29) if we lag the evaluation of $\mathbf{W}^{\mathrm{R}}$. Using a backward Euler formula for (27), the system (27)-(29) is integrated from time t_n to time $t_{n+1} = t_n + \Delta t$ via

$$\frac{1}{a_{n+1}\Delta t}\left(\bar{\mathbf{V}}'_{n+1} - \bar{\mathbf{V}}'_{n}\right) = \mathbf{R}^{\mathrm{T}}_{n+1} \cdot \mathbf{D}'_{n+1} \cdot \mathbf{R}_{n+1} - \bar{\mathbf{D}}'_{n+1}, \tag{30}$$

$$J_{n+1} = \exp\left(\mathrm{tr}\left(\mathbf{D}_n\right)\Delta t\right) J_n, \tag{31}$$

$$\mathbf{R}_{n+1} = \exp\left(\mathbf{W}^{\mathrm{R}}_n \Delta t\right)\mathbf{R}_n. \tag{32}$$

Implicit update of the deviatoric stretch tensor

With respect to $\bar{\mathbf{V}}'_{n+1}$, (30) is a nonlinear equation, since, from (24) and (19),

$$\begin{aligned}\bar{\mathbf{D}}'_{n+1} &= \frac{1}{2}\left[\bar{\mathbf{L}}(\bar{\boldsymbol{\tau}}_{n+1}) + \bar{\mathbf{L}}^{\mathrm{T}}(\bar{\boldsymbol{\tau}}_{n+1})\right] \\ &= \frac{1}{2}\left[\bar{\mathbf{L}}\left(\frac{2G}{a}\bar{\mathbf{V}}'_{n+1}\right) + \bar{\mathbf{L}}^{\mathrm{T}}\left(\frac{2G}{a}\bar{\mathbf{V}}'_{n+1}\right)\right].\end{aligned} \tag{33}$$

Writing (30) in the residual form

$$F\left(\bar{\mathbf{V}}'_{n+1}\right) \equiv \frac{1}{a_{n+1}\Delta t}\left(\bar{\mathbf{V}}'_{n+1} - \bar{\mathbf{V}}'_{n}\right) - \mathbf{R}^{\mathrm{T}}_{n+1}\cdot\mathbf{D}'_{n+1}\cdot\mathbf{R}_{n+1} + \bar{\mathbf{D}}'_{n+1} = 0, \tag{34}$$

we apply a Newton procedure to generate a sequence of approximations $\bar{\mathbf{V}}'^{(k)}_{n+1}$, $k = 1, 2, \ldots$, initialized by $\bar{\mathbf{V}}'^{(0)}_{n+1} = \bar{\mathbf{V}}'_{n}$:

$$\bar{\mathbf{V}}'^{(k+1)}_{n+1} = \bar{\mathbf{V}}'^{(k)}_{n+1} + \delta\bar{\mathbf{V}}'^{(k)}_{n+1} \tag{35}$$

where $\delta\bar{\mathbf{V}}'^{(k)}_{n+1}$ is the solution of

$$\left[\frac{\partial F}{\partial\bar{\mathbf{V}}'}\left(\bar{\mathbf{V}}'^{(k)}_{n+1}\right)\right]\delta\bar{\mathbf{V}}'^{(k)}_{n+1} = -F\left(\bar{\mathbf{V}}'^{(k)}_{n+1}\right), \tag{36}$$

whose coefficient matrix is the Jacobian

$$\frac{\partial F}{\partial\bar{\mathbf{V}}'}\left(\bar{\mathbf{V}}'^{(k)}_{n+1}\right) = \frac{1}{a_{n+1}\Delta t}\mathbf{I} + \frac{G}{a}\left[\frac{\partial\bar{\mathbf{L}}}{\partial\bar{\boldsymbol{\tau}}'}\left(\frac{2G}{a}\bar{\mathbf{V}}'^{(k)}_{n+1}\right) + \frac{\partial\bar{\mathbf{L}}^{\mathrm{T}}}{\partial\bar{\boldsymbol{\tau}}'}\left(\frac{2G}{a}\bar{\mathbf{V}}'^{(k)}_{n+1}\right)\right]. \tag{37}$$

The evaluation of (34) and (37) therefore requires $\bar{\mathbf{L}}$ and $\partial\bar{\mathbf{L}}/\partial\bar{\boldsymbol{\tau}}'$ evaluated at given values of $\bar{\boldsymbol{\tau}}'$, which is provided by the fine-scale model.

5 Fine-scale plasticity model

Given $\bar{\boldsymbol{\tau}}'$, the fine-scale model computes the strain rate

$$\bar{\mathbf{L}} = \bar{\mathbf{D}} = \dot{\gamma}_0 \sum_k s^{(k)}_{ij}\left(\frac{|s^{(k)}_{\alpha\beta}\bar{\boldsymbol{\tau}}'|}{g}\right)^m \operatorname{sgn}(s^{(k)}_{\alpha\beta}\bar{\boldsymbol{\tau}}'). \tag{38}$$

As described in [1], (38) is a summation over slip systems where the coefficients are computed using an iterative method involving fast Fourier transforms. This is a somewhat simplified version of the model described in [1], in which we have replaced the critical resolved shear stresses of the multiple systems with a uniform hardness parameter g that is updated by the fine-scale model and stored as a history variable $\mathcal{H} = \{g\}$. A constant, and still to be specified microstructure, is assumed.

6 Specification for the integration of the coupled coarse- and fine-scale systems over a time step

We now describe a step-by-step specification for the integration of the coupled multiscale system from time t_n to time $t_{n+1} = t_n + \Delta t$. We begin by assuming that all quantities are known at time t_n. Subscripts indicate the time at which quantities are evaluated, *e.g.*, $\rho_n \equiv \rho(t_n)$. A schematic diagram of the specification is contained in Figures 1 and 2.

Coarse-scale model update

Procedure C1: Given $\mathbf{x}_n$, $\mathbf{v}_n$, η_n, $\boldsymbol{\sigma}_n$, q_n and $\mathbf{L}_n$, integrate (1)-(7) from time $t = t_n$ to $t = t_{n+1}$, yielding $\mathbf{x}_{n+1}$, $\mathbf{v}_{n+1}$, η_{n+1} and e_{n+1}. Compute $q_{n+1} = q(\mathbf{v}_{n+1})$ and $\mathbf{L}_{n+1}$.

Procedure C2: Compute the new deviatoric stress $\boldsymbol{\sigma}'_{n+1} = \boldsymbol{\sigma}_{n+1} + (p_{n+1} + q(\mathbf{v}_{n+1}))\mathbf{I}$ using the stress $\boldsymbol{\sigma}_{n+1}$ obtained from Procedure K7(c) and pressure p_{n+1} obtained from Procedure K2(c).

Kinematic variable update

Procedure K1: Given $\mathbf{V}_n$, $\dot{\bar{\mathbf{V}}}'_n$, $\mathbf{R}_n$, $\mathbf{L}_n$, $\bar{\mathbf{L}}_n$ and $\mathbf{L}_{n+1}$,

(a) Set $\bar{\mathbf{V}}_n \equiv \mathbf{R}_n^{\mathrm{T}} \cdot \bar{\mathbf{V}} \cdot \mathbf{R}_n$,

(b) Set $J_n \equiv \det(\mathbf{V}_n)$,

(c) Set $a_n \equiv J_n^{1/3}$,

(d) Set $\mathbf{D}_m \equiv \frac{1}{2}\left(\mathbf{L}_m + \mathbf{L}_m^{\mathrm{T}}\right), \quad m = n, n+1$,

(e) Set $\bar{\mathbf{D}}_n \equiv \frac{1}{2}\left(\bar{\mathbf{L}}_n + \bar{\mathbf{L}}_n^{\mathrm{T}}\right)$,

(f) Set $\mathbf{W}_n \equiv \frac{1}{2}\left(\mathbf{L}_n - \mathbf{L}_n^{\mathrm{T}}\right)$,

(g) Set $\bar{\mathbf{W}}_n \equiv \frac{1}{2}\left(\bar{\mathbf{L}}_n - \bar{\mathbf{L}}_n^{\mathrm{T}}\right)$,

(h) Set
$$\begin{aligned}\mathbf{W}_n^{\mathrm{R}} &\equiv \dot{\mathbf{R}}_n \cdot \mathbf{R}_n^{\mathrm{T}} \\ &= \mathbf{W}_n - \mathbf{R}_n \cdot \bar{\mathbf{W}}_n \cdot \mathbf{R}_n^{\mathrm{T}} \\ &- \frac{1}{a_n}\mathbf{R}_n \cdot \left[\bar{\mathbf{V}}'_n \cdot \left(\bar{\mathbf{D}}'_n + \frac{1}{2a_n}\bar{\mathbf{V}}'_m\right) - \left(\bar{\mathbf{D}}'_n + \frac{1}{2a_n}\bar{\mathbf{V}}'_m\right) \cdot \bar{\mathbf{V}}'_n\right] \cdot \mathbf{R}_n^{\mathrm{T}}.\end{aligned}$$

Procedure K2: Integrate the kinematic system:

(a) Set $\mathbf{R}_{n+1} = \exp\left(\mathrm{tr}(\mathbf{W}_n^{\mathrm{R}})\Delta t\right)\mathbf{R}_n$,

(b) Set $J_{n+1} = \exp\left(\mathrm{tr}(\mathbf{D}_n)\Delta t\right) J_n$ and $a_{n+1} = J_{n+1}^{1/3}$,

(c) Compute p_{n+1} using Procedure K3,

(d) Solve

$$F(\bar{\mathbf{V}}'_{n+1}) \equiv \frac{1}{a_{n+1}\Delta t}\left(\bar{\mathbf{V}}'_{n+1} - \bar{\mathbf{V}}'_n\right) + \bar{\mathbf{D}}'_{n+1} - \mathbf{R}_{n+1}^{\mathrm{T}} \cdot \mathbf{D}'_{n+1} \cdot \mathbf{R}_{n+1} = 0 \qquad (39)$$

for $\bar{\mathbf{V}}'_{n+1}$ using Procedure K4.

Procedure K3: Set $p_{n+1} = p(e_{n+1}, J_{n+1})$ using (20).

Procedure K4: Perform a Newton iteration, using Procedure K5 to evaluate the Newton residual (34) and its corresponding Jacobian (37) and Procedure K6 to solve the Jacobian system.

Procedure K5: Given a Newton iterate $\bar{\mathbf{V}}'^{(k)}_{n+1}$, ($k$ is the iteration index),

(a) Set $\bar{\mathbf{E}}'^{(k)}_{n+1} = \frac{1}{a_{n+1}}\bar{\mathbf{V}}'^{(k)}_{n+1}$,

(b) Set $\bar{\boldsymbol{\tau}}'^{(k)} \equiv 2G\bar{\mathbf{E}}'^{(k)}_{n+1}$, where G is a constant shear modulus,

(c) Using $\bar{\boldsymbol{\tau}}'^{(k)}$, get $\bar{\mathbf{L}}$ and $\partial\bar{\mathbf{L}}/\partial\bar{\boldsymbol{\tau}}'$ using Procedure K1,

(d) Set $\bar{\mathbf{D}}^{(k)}_{n+1} \equiv \bar{\mathbf{L}}$,

(e) Evaluate (34) and (37).

Procedure K6: Solve (36).

Procedure K7: Given the solution $\bar{\mathbf{V}}'_{n+1}$ of the Newton solve,

(a) Set $\bar{\boldsymbol{\tau}}_{n+1} = (p_{n+1} + q_{n+1})\mathbf{I} + \frac{2G}{a_{n+1}}\bar{\mathbf{V}}'_{n+1}$,

(b) Set $\bar{\boldsymbol{\sigma}}_{n+1} = J^{-1}_{n+1}\bar{\boldsymbol{\tau}}_{n+1}$,

(c) Set $\boldsymbol{\sigma}_{n+1} = \mathbf{R}_{n+1} \cdot \bar{\boldsymbol{\sigma}}_{n+1} \cdot \mathbf{R}^{\mathrm{T}}_{n+1}$.

Fine-scale model evaluation

Procedure F1: Evaluate $\bar{\mathbf{L}}$ and its $\bar{\boldsymbol{\tau}}$ derivative using adaptive sampling and update the history $\mathcal{H}$, which consists solely of the hardness parameter g.

Procedure F2: Query the interpolation model database for the k^{th} nearest neighbors to $(\bar{\boldsymbol{\tau}}_{n+1}, g)$ based on a prescribed tolerance.

Procedure F3: If the set of nearest neighbor interpolation models is non-empty, use the interpolation models to interpolate $\bar{\mathbf{L}}$ and its derivative at $(\bar{\boldsymbol{\tau}}_{n+1}, g)$. Compute the error estimate.

Procedure F4: If the error tolerance is exceeded, or no interpolation models are close enough, call VPFFT to compute a new $\bar{\mathbf{L}}$ and g. Otherwise, return $\bar{\mathbf{L}}$ and its derivative.

Procedure F5: Add the new fine-scale evaluation to an existing model in the nearest neightbor set. Otherwise, create a new model. Update the database with the new objects created in either case.

Procedure F6: Use the interpolation model to compute the derivative $\partial\bar{\mathbf{L}}/\partial\bar{\boldsymbol{\tau}}$.

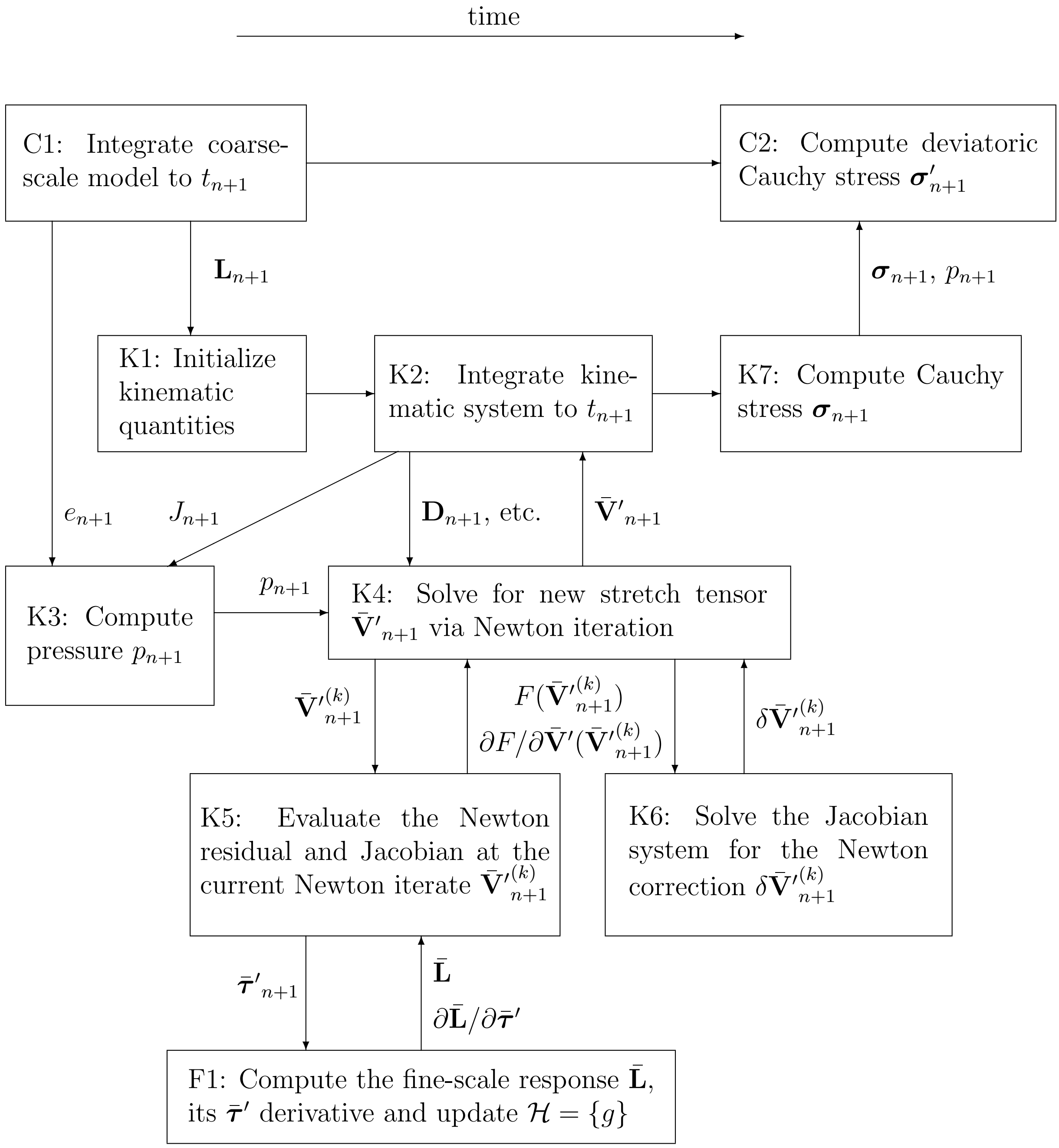

Figure 1: Coupled integration schematic (Part I).

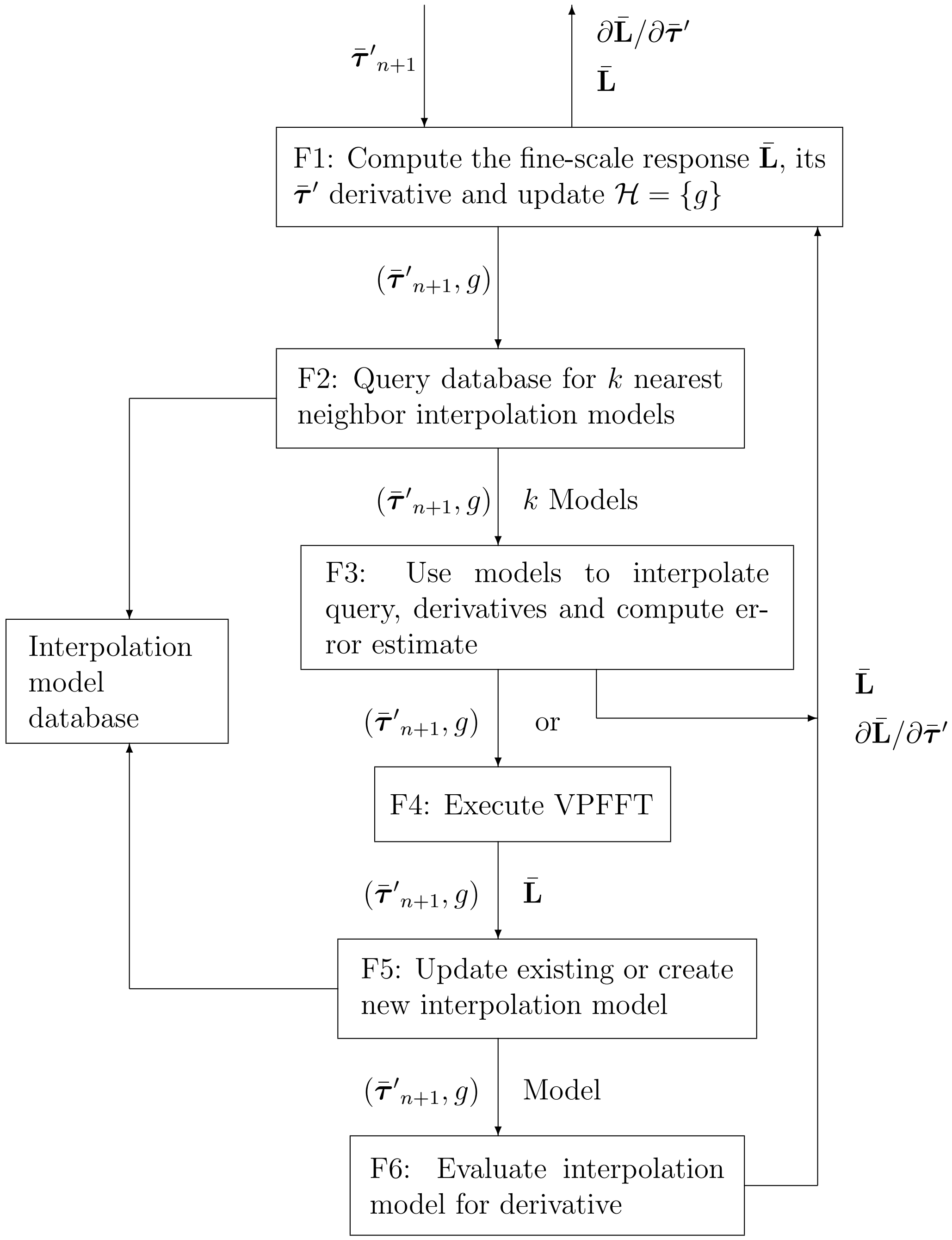

Figure 2: Coupled integration schematic (Part II).

7 Adaptive sampling database objects

Evaluation of the stress tensor $\boldsymbol{\sigma}$ at each time step at all of the quadrature points used in the finite element discretization implies a large number of fine-scale model calculations. As described in the fine-scale model evaluation part of the previous section, adaptive sampling attempts to significantly reduce the number of fine-scale evaluations by dynamically constructing a database of interpolation models based on previous fine-scale evaluations. The objects stored in the database used by the database consist not only of fine-scale model evaluations, but also certain interpolation coefficients constructed by the kriging interpolation algorithm. To define these precisely, we summarize the kriging algorithm used in the ASPA proxy app.

Summary of univariate kriging algorithm

Kriging is a type of scattered data interpolation first developed in the field of geostatistics. Given a set of experimental measurements, the goal is to estimate the response at points for which no measurements exist. Rather than basing the interpolant simply on some measure of the distance to known points, kriging interpolation attempts to also incorporate information about data correlation. If, for example, a large number of experimental observations exist in a small region, it is possible that the data is sufficiently correlated that much of it is redundant. Depending upon the interpolation goals, failure to account for the correlation of clustered data could potentially result in undesirable over-weighting. The estimation of data correlation is therefore conducted as a precursor to kriging interpolation, involving, for example, the creation of a variogram.

Kriging interpolation assumes that, over some region $\Omega \subset \mathbb{R}^D$, the function being interpolated can be expressed as the sum of a regression (a.k.a. trend) model and a stochastic deviation

$$s(\mathbf{x}) = m(\mathbf{x}) + Z(\mathbf{x}), \tag{40}$$

where $Z(\mathbf{x})$ is assumed to have zero mean and covariance of the form

$$Cov\left\{Z(\mathbf{x}, \mathbf{w})\right\} = \sigma^2 R(\mathbf{x}, \mathbf{w}) \tag{41}$$

with σ^2 denoting the process variance. Typically, a linear regression model

$$m(\mathbf{x}) = \mathbf{p}^{\mathbf{T}}(\mathbf{x})\beta \tag{42}$$

is assumed, where the components of $\mathbf{p}(\mathbf{x}) \equiv [\mathbf{p}_1(\mathbf{x}), \mathbf{p}_2(\mathbf{x}), \ldots, \mathbf{p}_D(\mathbf{x})]$ form a basis for the space of linear mappings of Ω into $\mathbb{R}$ and $\beta \in \mathbb{R}^D$ is a vector of regression coefficients. Given known values of s at points $\mathbf{x}_i \in \Omega$, $i = 1, \ldots, N$, the kriging interpolant is defined as

$$\hat{s}(\mathbf{x}) \equiv m(\mathbf{x}) + \sum_{i=1}^{N} \lambda_i(\mathbf{x})(s(\mathbf{x}_i) - m(\mathbf{x}_i)), \quad \mathbf{x} \in \Omega, \tag{43}$$

where the coefficients $\lambda_i(\mathbf{x})$ are chosen to minimize the error variance

$$\begin{aligned} Var(\hat{s}(\mathbf{x}) - s(\mathbf{x})) &= Var\{\hat{s}(\mathbf{x}) - m(\mathbf{x}) - (s(\mathbf{x}) - m(\mathbf{x}))\} \\ &= Var\left\{\sum_{i=1}^{N} \lambda_i(\mathbf{x})(s(\mathbf{x}_i) - m(\mathbf{x}_i))\right\} + Var\left\{s(\mathbf{x}) - m(\mathbf{x})\right\} \\ &\quad - 2Cov\left\{\sum_{i=1}^{N} \lambda_i(\mathbf{x})(s(\mathbf{x}_i) - m(\mathbf{x}_i)), s(\mathbf{x}) - m(\mathbf{x})\right\} \\ &= \sigma^2 \left(\sum_{i=1}^{N}\sum_{j=1}^{N} \lambda_i(\mathbf{x})\lambda_j(\mathbf{x}) R(\mathbf{x}_i, \mathbf{x}_j) + 1 - 2\sum_{i=1}^{N} \lambda_i(\mathbf{x}) R(\mathbf{x}_i, \mathbf{x})\right), \end{aligned} \tag{44}$$

subject to the constraint

$$\mathbf{p}(\mathbf{x}) - \sum_{i=1}^{N} \lambda_i(\mathbf{x})\mathbf{p}(\mathbf{x_i}) = 0. \tag{45}$$

The condition (45) ensures that the error expectation $E\{\hat{s}(\mathbf{x}) - s(\mathbf{x})\}$ vanishes independently of the regression coefficients β. By introducing Lagrange multipliers corresponding to (45), the resulting unconstrained minimization problem is solved by finding the critical point of the augmented system. The result is [4]

$$\lambda(\mathbf{x}) \equiv [\lambda_1(\mathbf{x}), \lambda_2(\mathbf{x}), \ldots, \lambda_N(\mathbf{x})] = \mathbf{r^T}(\mathbf{x})\mathbf{R}^{-1}, \tag{46}$$

$$\beta \equiv [\beta_1, \beta_2, \ldots, \beta_D] = \left(\mathbf{P^T}\mathbf{R}^{-1}\mathbf{P}\right)^{-1} \mathbf{P^T}\mathbf{R}^{-1}\mathbf{v}, \tag{47}$$

where $\mathbf{v} \equiv [s(\mathbf{x}_1), s(\mathbf{x}_2), \ldots, s(\mathbf{x}_N)]$ is the vector of known data,

$$\mathbf{P} \equiv \begin{bmatrix} p_1(\mathbf{x}_1) & \ldots & p_D(\mathbf{x}_1) \\ \ldots & \ddots & \ldots \\ p_1(\mathbf{x}_N) & \ldots & p_D(\mathbf{x}_N) \end{bmatrix}, \tag{48}$$

$$\mathbf{R} \equiv \begin{bmatrix} 1 & R(\mathbf{x}_1, \mathbf{x}_2) & \ldots & R(\mathbf{x}_1, \mathbf{x}_N) \\ R(\mathbf{x}_2, \mathbf{x}_1) & 1 & \ldots & R(\mathbf{x}_2, \mathbf{x}_N) \\ \ldots & \ldots & \ddots & \ldots \\ R(\mathbf{x}_N, \mathbf{x}_1) & \ldots & R(\mathbf{x}_N, \mathbf{x}_{N-1}) & 1 \end{bmatrix}, \tag{49}$$

and

$$\mathbf{r}(\mathbf{x}) \equiv \begin{bmatrix} R(\mathbf{x}_1, \mathbf{x}) \\ \ldots \\ R(\mathbf{x}_N, \mathbf{x}) \end{bmatrix}. \tag{50}$$

Database object size estimation

In the present context of our elastoviscoplasticity proxy app, the independent variable $\mathbf{x}$ is the tuple $(\bar{\boldsymbol{\tau}}', g)$ comprised of the deviatoric component of the Kirchoff stress and the hardness parameter. The dimension of the query space is therefore $D = 9$. The function being interpolated is $\bar{\mathbf{L}}$, which, due to symmetry, has six degrees of freedom. Taking into account the fact that this interpolation is multivariate, an interpolation object contains

1. The points $\mathbf{x}_i = (\bar{\boldsymbol{\tau}}'_i, g_i)$, $i = 1, \ldots, N$, at which the fine-scale model has been previously evaluated (9N doubles).

2. The fine-scale evaluations (6N doubles)

$$\mathbf{v} = [s(\mathbf{x}_1), s(\mathbf{x}_2), \ldots, s(\mathbf{x}_N)] = [\bar{\mathbf{L}}(\bar{\boldsymbol{\tau}}'_1, g_1), \bar{\mathbf{L}}(\bar{\boldsymbol{\tau}}'_1, g_2), \ldots, \bar{\mathbf{L}}(\bar{\boldsymbol{\tau}}'_N, g_N), \tag{51}$$

3. The regression coefficients β defined by (47) (6N doubles),

4. The inverses of the matrices $\mathbf{R}$ and $\mathbf{P^TR^{-1}P}$ $((6N)^2 + (6N^2) = 72N^2$ doubles),

The total number of doubles in a database object is therefore $21N + 72N^2$.

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