PETSc finite element details

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1 Weak form PDEs

Consider a strong form PDE with fields u_0, u_1, \ldots , each of which has components u_{i0}, u_{i1}, \ldots , and equations

 $f_{ab}\left(u_{ij},\partial_k u_{ij},\partial_k\partial_l u_{ij}\right) = 0$

where we have one f_{ij} for each u_{ij} . We use the convention that an index occurring only inside a function call means that all values of the index are passed to the function. When we later discretize over space, u_i and u_j will be allowed to live in different discrete function spaces, while u_{ij} and u_{ik} come the same function space.

We pass to the weak form by integrating a smooth test function v_{ab} against f_{ab} , then integrating by parts to get

$$\int_{\Omega} v_{ab} f_{ab} \left(u_{ij}, \partial_k u_{ij}, \partial_k \partial_l u_{ij} \right) dx = 0$$
$$\int_{\Omega} v_{ab} f_{ab}^0 \left(u_{ij}, \partial_k u_{ij} \right) dx + \int_{\Omega} \partial_c v_{ab} f_{abc}^1 \left(u_{ij}, \partial_k u_{ij} \right) dx = 0$$

where f^0 and f^1 depend on u only to first derivatives. The pointwise functions f^0 and f^1 are exposed to petsc, with u_{ij} passed as an (i, j)-major array and $\partial_k u_{ij}$ as an (i, j, k)-major array. f^0_{ab} is split into functions f^0_a each returning a *b*-major array, and f^1_{abc} is split into functions f^1_a each returning a (b, c)-major array. In weird pseudocode signatures,

```
#define AUX a[i,j], da[i,j]/dx[k], x[k]
f0[a] : (u[i,j], du[i,j]/dx[k], AUX) -> [b];
f1[a] : (u[i,j], du[i,j]/dx[k], AUX) -> [b,c];
```

where x_k is position and a_{ij} are auxiliary fields.

2 Boundary conditions

With boundary conditions, the weak form of the PDE becomes

$$\int_{\Omega} v_{ab} f_{ab}^0 dx + \int_{\Omega} \partial_c v_{ab} f_{abc}^1 dx + \int_{\delta\Omega} v_{ab} f_{ab}^{0\partial} da + \int_{\delta\Omega} \partial_c v_{ab} f_{abc}^{1\partial} da = 0$$

where the boundary condition terms $f^{0\partial}$ and $f^{1\partial}$ additionally depend on outward pointing boundary normals n_k . The pseudocode signatures are the same as for f^0 and f^1 except for the dependence on normals:

3 Jacobians

The above is sufficient for computing residuals. For residual Jacobians, we additionally need first derivatives of f^0 and f^1 w.r.t. u and ∇u , for a total of four additional functions g^0, g^1, g^2, g^3 . Theoretically we might also need derivatives of the boundary terms, but this is currently unsupported.

We split the 4-valued indexed g^{γ} into $g^{\alpha\beta}$ where $\gamma = 2\alpha + \beta$. $g^{\alpha\beta}$ represents the Jacobian of f^{α} w.r.t. the β th derivatives of u:

$$g_{aibj}^{00} = \frac{d}{du_{ij}} f_{ab}^{0}$$
$$g_{aibjk}^{01} = \frac{d}{d\partial_k u_{ij}} f_{ab}^{0}$$
$$g_{aibcj}^{10} = \frac{d}{du_{ij}} f_{abc}^{1}$$
$$g_{aibcjk}^{11} = \frac{d}{d\partial_k u_{ij}} f_{abc}^{1}$$

Each $g^{\alpha\beta}$ is split into a two dimensional array of functions $g_{ai}^{\alpha\beta}$ giving function f_a^{α} differentiated against the β th derivatives of u_i . In signatures:

g^{00}[a,i] : (...) -> [bj]; g^{01}[a,i] : (...) -> [bjk]; g^{10}[a,i] : (...) -> [bcj]; g^{11}[a,i] : (...) -> [bcjk];