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(U) Weighted condition number relaxation with discrete weights

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Abstract

The extension of the condition number mesh relaxer to allow arbitrary discretely defined weights is discussed. A convolution approach, allowing careful control of the gradient and Hessian of the reconstructed weight function is used. Approximations for the calculation of the convolution integrals to enable useful application in ALE codes are explored.

Overview

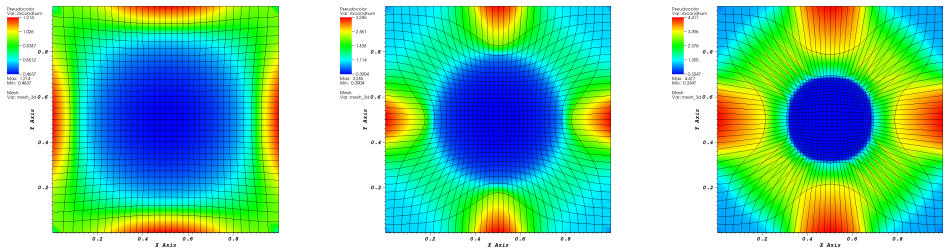
In arbitrary Lagrangian-Eulerian (ALE) calculations, there is often a desire to dynamically move the mesh towards regions of interest. This is specified using weights that can be a function of material or state (i.e. artificial viscosity, equivalent plastic strain, etc). The mesh relaxer can then dynamically adapt the mesh to provide enhanced resolution near features of interest. In staggered grid hydrodynamics, the relaxation weight variables are usually defined as piece-wise constant over a zone giving rise to a discontinuous field. This work is motivated by the extension of the condition number relaxer to support discrete defined weights in ALE calculations.

Condition number relaxation

The condition number (CN) relaxer, developed by P. Knupp [1, 2, 3], is expressed in the minimization of an objective functional composed of the contributions from each corner of each element. In 2D, a corner in an element centered at node i, will consist of two adjacent edges, $\mathbf{e_{ik}}$ and $\mathbf{e_{ik}}$. In 3D, it consists of three edges with a common vertex ordered as a right hand system. The resulting functionals in 2D and 3D are given in Eqn. 1.

$$F_{i,j,k} = \frac{|\mathbf{e_{ij}}|^2 + |\mathbf{e_{ik}}|^2}{|\mathbf{e_{ij}} \times \mathbf{e_{ik}}|}, \quad F_{i,j,k,l} = \frac{|\mathbf{e_{ij}}|^2 + |\mathbf{e_{ik}}|^2 + |\mathbf{e_{il}}|^2}{|(\mathbf{e_{ij}} \times \mathbf{e_{ik}}) \cdot \mathbf{e_{il}}|^{\frac{2}{3}}} \tag{1}$$

Each relaxation step is the application of one or more iterations of a Newton minimization procedure, for



$\gamma = 4$ $\gamma = 16$ $\gamma = 64$

Figure 1: Weighted condition number relaxation using analytic weighting function $W = \tanh\left(\gamma \|\mathbf{x} - \mathbf{x}_0\|\right) + 2$

example in 2D,

$$\mathbf{x}_i^{n+1} = \mathbf{x}^n - \begin{pmatrix} \frac{\partial^2 F}{\partial x_i^2} & \frac{\partial^2 F}{\partial x_i \partial y_i} \\ \frac{\partial^2 F}{\partial x_i \partial y_i} & \frac{\partial^2 F}{\partial y_i^2} \end{pmatrix}^{-1} \begin{pmatrix} \frac{\partial F}{\partial x_i} \\ \frac{\partial F}{\partial y_i} \end{pmatrix} \tag{2}$$

where $F = \sum_i F_{i,i+1,i+2,i+3}$.

An extension to a weighted version was developed by Vachal et. al [4]. In this formulation, the objective functional is modified as

$$F'_{i,j,k} = \frac{1}{W_i} F_{i,j,k} \tag{3}$$

where W_i is the corner weight function. Obviously to apply the minimization procedure in Eqn. 2 using the weighted functional, the first and second partial derivatives of the weighting function must be defined and available. In Vachal, only analytic expressions were used. This work is focused on the robust extension of the method to the use of discretely defined and, in general, discontinuous weighting functions.

In a motivating example, shown in Fig. 1, the performance of the weighted CN relaxer as described by Vachal et. al. with analytic weighting functions depends primarily on the local gradient and Hessian of the weight function. Even though the nominal values of the weights are the same in each calculation, the relaxation performance strongly depends on the transition interval between the two limiting values where the gradient and Hessian of the weight function vary strongly.

For discretely defined weights a twice differentiable reconstruction is required but as illustrated, tight control over the derivatives is needed and this cannot be achieved with classical piece-wise parabolic type reconstruction methods.

Discrete Weights Reconstruction Strategy

For purposes of the weighted relaxation strategy, the reconstruction procedure used to obtain a C^2 representation of the weighting function has a few requirements. However, *it need not be interpolatory* in

that in does not need to match the mean values over each element nor does it have to attain a specific point value. It should, however, be

1. Locally computable along with first and second derivatives,
2. Respect the weights in a general sense,
3. Be a reasonable average of the weights of the connected elements at a node.

The approach taken here is to calculate a mollified weight function using a convolution of the discrete weights with a smoothing function. That is, at a node, the local representation of the smoothed weight function is defined as

$$\left(\frac{2}{\sqrt{\pi}}\right)^d \left(\frac{1}{(ch)^2}\right) \iiint_{-\infty}^{\infty} W_i(\xi,\eta,\zeta) \exp\left(-\frac{1}{(ch)^2}\left((x-\xi)^2+(y-\eta)^2+(z-\zeta)^2\right)\right) d\xi\, d\eta\, d\zeta \quad (4)$$

where $W_i(\xi,\eta,\zeta)$ are the piece-wise constant, element centered weights. Ultimately we wish to evaluate Eqn. 4 at each node. The smoothing function is effectively zero outside a small radius of the node, allowing the restriction of the the domain of integration to the union of all elements containing the node $\mathbf{x}_i$.

For the specific case of a structured block of elements, the mollified weighting function is readily computable. The contribution of an element with domain $[x_a, x_b] \times [y_a, y_b]$ is

$$\begin{aligned}\frac{1}{4(ch)^2} W_i \left(\int_{x_a}^{x_b} \frac{2}{\sqrt{\pi}} \exp\left(-\frac{1}{(ch)^2}(x-\xi)^2\right) d\xi\right) \left(\int_{y_a}^{y_b} \frac{2}{\sqrt{\pi}} \exp\left(-\frac{1}{(ch)^2}(y-\eta)^2\right) d\eta\right) \\ = \frac{W_i}{4}\left\{erf\left(\frac{1}{(ch)^2}(x_b-x)\right) - erf\left(\frac{1}{(ch)^2}(x_a-x)\right)\right\} \\ \cdot \left\{erf\left(\frac{1}{(ch)^2}(y_b-y)\right) - erf\left(\frac{1}{(ch)^2}(y_a-y)\right)\right\} \quad (5)\end{aligned}$$

The reconstructed or mollified continuous, differentiable weight function for a four element block is shown in Fig. 2 with different values of the smoothing length. For small smoothing lengths, there is a sharp transition. Note, that for the convolution integral to remain "local" to the element patch, the smoothing length has to be such that it is significantly smaller than the characteristic local mesh length scale. In particular, c should be small, likely less than 0.25.

Radially symmetric approximation

For a distorted grid, the convolution is not available analyticly. However, approximations may be made to make evaluation computationally tractable. High order quadrature is possible, but initial tests showed quadrature rules of order 16 or higher may be required for acceptable results making it impractical for ALE use.

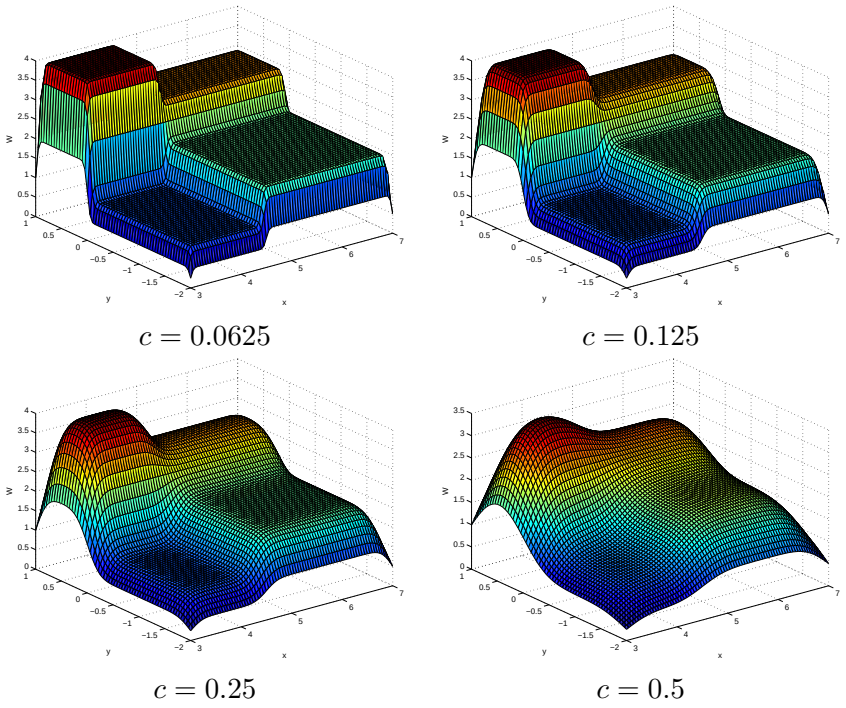


Figure 2: Analytic mollified weighting function with four different values for the smoothing width. The local length scale h was taken to be 1

However, in 2D the convolution integral is radially symmetric, up to the variation in the discrete weights. Taking the origin as the vertex of the current corner in the calculation, the variation in the weights can be regarded as a function of only θ, the angle relative to a reference edge, by extending the edges to ∞. With this approximation, the value of the condition number functional and its derivatives are readily computable in 2D and closed form expressions obtained. On going work is extending this, or obtain alternate approximations for 3D.

$$\frac{1}{4(ch)^2}\left(\frac{2}{\sqrt{\pi}}\right)^2 \iint_{-\infty}^{\infty} W_i(\xi,\eta)\exp\left(-\frac{1}{(ch)^2}\left((x-\xi)^2+(y-\eta)^2\right)\right) d\xi\, d\eta$$
$$= \frac{1}{4(ch)^2}\int_0^{2\pi} W_i(\theta)\int_0^{\infty}\exp\left(-\frac{r^2}{(ch)^2}\right) r\, dr\, d\theta = \sum_k W_k(\theta^{k^+}-\theta^{k^+}) \quad (6)$$

where θ^{k^+} and θ^{k^+}) are the angle of the edge with respect to a vector aligned with the x-axis.

The gradient terms are likewise computed:

$$\frac{\partial W_k}{\partial x} = \sum_k W_k(\sin\ \theta^{k^+} - \sin\theta^{k^-})$$
$$\frac{\partial W_k}{\partial x} = -\sum_k W_k(\cos\ \theta^{k^+} - \cos\theta^{k^-})$$

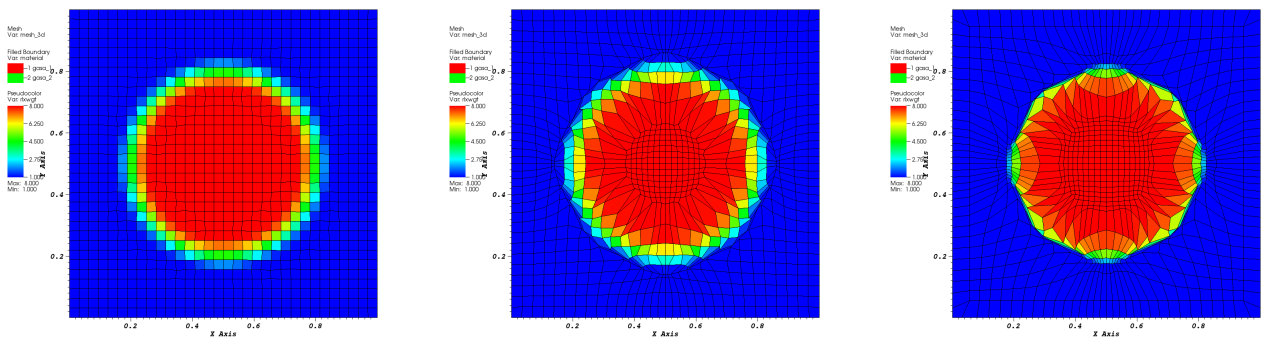
The discrete weights are element based and smoothed. The weight function for a corner is taken to be the weight function for the central node (unlike the average in Vachal, et. al). An example calculation is shown in Fig. 3. Unlike with the analytic weighting function, the discrete version has the weights changing in time as they are treated as field variables and subject to remap. The discrete version shows considerable sensitivity to the smoothing length, c, and generally inhibits the robustness of the CN relaxer.

Conclusions

A possible formulation for weighted condition number relaxation with discrete weights has been developed. However,

- the weighted versions of the relaxer are generally less robust,
- there is still considerable sensitivity to the gradient of the reconstructed weight function motivating alternate objective function formulations that only depend on the ratio of weights,
- the extension to 3D is not trivial.

Current efforts are on other extensions of the CN functional.



Initial Weights $c = 0.25$ $c = 0.5$

Figure 3: Discretely weighted condition number relaxer after 100 cycles of smoothing.

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