Legend:

- **Complete item**
- **Incomplete item**

6-22-2015

1. **Obtain multidimensional results for explicit FCT.**

   See the results document.

2. **Compare symmetric limiter with upwind limiter.**

   The symmetric limiting coefficients have the following definition:

$$L_{i,j} = \begin{cases} \min\{R_i^+, R_j^-\}, & F_{i,j} > 0 \\ \min\{R_i^-, R_j^+\}, & F_{i,j} < 0 \end{cases}, \tag{1}$$

   while the upwind-biased limiting coefficients have the following definition:

$$L_{i,j} = \begin{cases} R_k^+, & F_{i,j} > 0 \\ R_k^-, & F_{i,j} < 0 \end{cases}, \tag{2}$$

   where k is the upwind node of i and j. It is noted here that, unlike the symmetric limiting coefficients, the upwind-biased limiting coefficients do not necessarily satisfy the discrete maximum principle. This is disproved here by a counterexample. Recall that the discrete maximum principle is satisfied when $Q_i^- \leq \sum_j L_{i,j} F_{i,j} \leq Q_i^+$. Suppose a node i has a single neighboring node $i-1$, and that this neighbor is upwind of i. For example, this is the case for a 1-D domain on the outflow boundary. Thus there is a single correction flux $F_{i,i-1}$: $\sum_j L_{i,j} F_{i,j} = L_{i,i-1} F_{i,i-1}$. Now suppose that without limitation, this correction flux would exceed the upper bound Q_i^+, i.e., $F_{i,i-1} > Q_i^+$. Suppose further that $P_{i-1}^+ \leq Q_{i-1}^+$. Then,

$$\sum_j L_{i,j} F_{i,j} = L_{i,i-1} F_{i,i-1} = R_{i-1}^+ F_{i,i-1} = \min\left\{1, \frac{Q_{i-1}^+}{P_{i-1}^+}\right\} F_{i,i-1} = F_{i,i-1} > Q_i^+,$$

   which violates the DMP condition. However, this limiting coefficient has yet to be tested for its effectiveness in practice.

3. **Determine if converged steady-state results match transient results.**

   In progress.

4. **Determine how to evaluate analytic DMP bounds in multidimensional problems.**

   In progress.

5. **Compare time step size computed from $\Delta t \leq \frac{m_i}{A_{i,i}^L}$ to that obtained by examining the eigenvalues of $(\mathbf{M}^L)^{-1}\mathbf{A}^L$.**

The condition $\Delta t \leq \frac{m_i}{A^L_{i,i}}$ results from the need to prove positivity of the low-order system matrix diagonal entries. The suggested approach of using the eigenvalues of $(\mathbf{M}^L)^{-1}\mathbf{A}^L$ is unclear. For a general scalar conservation law

$$u_t + \mathbf{f}(u)_x = 0,$$

the equation may be expressed using chain rule:

$$u_t + \frac{d\mathbf{f}}{du}u_x = 0,$$

where $\frac{d\mathbf{f}}{du}$ is the characteristic speed [2]. In the case of a discrete FEM system

$$\mathbf{M}\mathbf{U}_t + \mathbf{A}(\mathbf{U})\mathbf{U}_x = 0,$$

the characteristic speeds would indeed be given by the eigenvalues of $\mathbf{M}^{-1}\mathbf{A}(\mathbf{U})$. However, this equation does not correspond to the system in question:

$$\mathbf{M}\mathbf{U}_t + \mathbf{B}(\mathbf{U})\mathbf{U} = 0,$$

and thus the suggestion is unclear. Expressing the system in question in the quasilinear form with the spatial derivative, i.e., expressing $\mathbf{B}(\mathbf{U})\mathbf{U}$ as $\mathbf{A}(\mathbf{U})\mathbf{U}_x$, is complicated by the presence of a reaction term and an artificial diffusion term. For instance, the governing equation would be

$$u_t + \mathbf{v}u_x + \sigma u = (\nu u_x)_x,$$

which in conservative form gives

$$\mathbf{f}(u) = \mathbf{v}u + \int \sigma u dx - \nu u_x,$$

and thus computing $\mathbf{f}'(u)$ is unclear.

An alternative approach to computing a valid time step size for the high-order scheme is therefore suggested here, at least in regards to the presence of the reaction term, not the viscosity term: the presence of a reaction term should only decrease the flux speed, a conservative time step size could be computed by ignoring the reaction term. Of course, when entropy viscosity is used, the flux speed is increased and thus the same reasoning cannot be applied. In general, a CFL-satisfying time step size can be computed by satisfying the following condition:

$$\Delta t^{n+1} \leq \frac{h_{min}}{s^n_{max}},$$

where h_{min} is the smallest element diameter in the mesh, and s^n_{max} is the largest flux speed computed in the domain. Calling s^{void} the flux speed computed when ignoring the reaction term, the following is true, as discussed before: $s^{void} \geq s$. Thus the usage of this flux yields a conservative time step estimate:

$$\Delta t^{n+1} \leq \frac{h_{min}}{s^{void,n}_{max}} \leq \frac{h_{min}}{s^n_{max}}.$$

6. **In the source-void-to-absorber problem, ramp the source from zero instead of instantaneously adding the source.**

   In progress.

7. **Determine if Kuzmin's implicit bounds are equivalent to our implicit bounds.**

   In [1], Kuzmin defines the limited flux bounds as

$$Q_i^{\pm} = m_i \overset{\max_j}{\underset{\min_j}{\max}} \left\{0, \tilde{U}_j - \tilde{U}_i\right\},$$

   where $\tilde{\mathbf{U}}$ is the "auxiliary" solution, given by Equations (75) and (69) in [1], which together give, in our notation (and adding a source term),

$$\mathbf{M}^L \frac{\tilde{\mathbf{U}} - \mathbf{U}^n}{(1-\theta)\Delta t} + \mathbf{A}^L \mathbf{U}^n = \mathbf{b}^n.$$

   This auxiliary solution can thus be interpreted as the low-order solution at time $t^{n+1-\theta}$, or alternatively may be viewed as the "explicit portion" of a low-order time step; for explicit Euler, this is the entire time step and thus $\tilde{\mathbf{U}} = \mathbf{U}^{L,n+1}$, while for implicit Euler, this includes none of the step and thus $\tilde{\mathbf{U}} = \mathbf{U}^n$. Thus the question of whether Kuzmin's implicit bounds are equivalent to ours is immediately answered: *they are not equivalent* because our implicit bounds are implicit with the new solution, while Kuzmin's are explicit.

   It should be noted that at least in [1], Kuzmin's objective appears to be to satisfy the positivity constraint given by Equation (83) in [1], unlike our objective, which is to satisfy a discrete maximum principle, which happens to have a lower bound greater than or equal to zero.

8. **Evaluate the benefit of Kuzmin's "prelimiting" step.**

   Equation (84) of [1] gives Kuzmin's prelimiting step:

$$F_{i,j} := 0 \qquad \text{if} \quad F_{i,j}\left(\tilde{U}_i - \tilde{U}_j\right) \leq 0,$$

   See the results document, which has a section on the effect of prelimiting. Prelimiting seems to have very little effect.

9. **For the defect correction scheme, try damping viscosity updates.**

   The implicit scheme is nonlinear and thus requires some iteration; the defect correction technique was used. It was noted that difficulties were noted in iteratively computing the entropy viscosity solution because entropy viscosity was oscillating between two states on each iteration. Thus a damping coefficient λ was applied to solution updates:

$$\mathbf{U}^{H,n+1,(k+1)} = \mathbf{U}^{H,n+1,(k)} + \lambda \Delta \mathbf{U}^{H,n+1,(k+1)}.$$

   This was found to give some success but still showed difficulties for some problems. It was thus suggested to try instead dampening only the entropy viscosity updates:

$$\nu^{E,n+1,(k+1)} = \nu^{E,n+1,(k)} + \lambda \Delta \nu^{E,n+1,(k+1)}.$$

6-23-2015

1. **Determine why Kuzmin needs defect correction if his limiting coefficients are explicit.** While answering the question of whether Kuzmin's implicit discrete maximum principle bounds were equivalent to ours, the question arose of why Kuzmin would need defect correction when his $Q_i^{\pm}$ are explicitly computed, since the resulting system is linear.

   In Section 6.1 of [1], Kuzmin mentions that the system matrices may depend on the solution if the velocity field does but that for brevity, the dependence of the solution on the matrices would be omitted. He then goes to introduce the defect correction scheme to resolve the nonlinearities in the governing equation and/or discretization procedure.

   In addition, in Section 6.2 of [1], Kuzmin states that artificial diffusion is proportional to time step size while the amount of acceptable antidiffusion depends solely on the local extrema of the auxiliary solution $\tilde{u}$. Thus, a smaller percentage of the available antidiffusion is accepted as the CFL number increases. He then proposes an iterative procedure to circumvent this problem. This has not yet been tested.

2. **Try a near-void instead of an actual void in the source-void-to-absorber test problem.**

   The physical solution for the source-void-to-absorber problem is linear in the void, followed by exponential decay. It was considered suspicious that the numerical solution in this region without artificial dissipation results in spurious oscillations, so it was suggested to try using very small σ in this region instead of $\sigma = 0$.

3. **Try a three-region problem.** See the results document.

4. **Try a two-region problem with equal saturation values but different values for q and σ.** If the saturation value of q/σ is reached in the first region, one would like to ensure that if the second region has the same saturation value q/σ, but different values of q and σ, then there should be no numerical artifacts at the interface between the two regions.

   See the results document. There appears to be a very small numerical artifact at the interface.

7-21-2015

I met with Dr. Ragusa, and John Peterson and David Andrs of the MOOSE team to discuss the possibility of implementing our FCT scheme in MOOSE. John outlined the main challenges of implementation to be the following:

- MOOSE currently can store only *one* matrix, whereas the FCT algorithm, as it is currently formulated, requires the storage of several matrices.
- MOOSE currently can only do one solve instead of the two solves per time step required by FCT (the first for the high-order solution and the second for the FCT solution).

It was suggested that perhaps the FCT algorithm may be formulated to allow matrix entries to be used on-the-fly and thus not stored. The possibility of creating "auxiliary" matrices to be used was expressed. Other concerns that were discussed include the end project goal:

- What is the goal to be completed by the end of my anticipated graduation/disseration (May 2016)?

- Is the end goal to be able to apply FCT to general conservation law *systems* or just general *scalar* conservation laws?
- Is the end goal to have these abilities in MOOSE or to have this capability somewhere (such as in `deal.II`)?

It was suggested that if the end goal is to apply FCT to *systems* that we should develop the theory for systems first and perhaps even write the systems code in `deal.II` since MOOSE currently lacks the ability to use FCT in its current formulation. Also it was suggested that it would be advantageous to write this `deal.II` code in parallel to expose any parallelization challenges.