10.34, Numerical Methods Applied to Chemical Engineering
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**Lecture #33: Operator Splitting. Strang Splitting.**

## *Problem Set 11*

$$\frac{t}{\tau} = -\ln(rand)$$

$$e^{-t/\tau} \approx rand \longleftarrow$$ Poisson Statistics

Poisson statistics can be found in applications such as radioactive decay, droplets hitting a roof, and average time between uncorrelated events.

Gillespie Algorithm – Must run many times
Continuum view: assume Poisson statistics

$t_{failure} = -\tau_{failure} \ln(rand)$ The $\tau_{failure}$ is from the continuum equations.

## *Operator Splitting*

### Problem

$\hat{A}$ and $\hat{B}$ have no time derivative.

$$\frac{\partial y}{\partial t} = (\hat{A}y) + (\hat{B}y) \qquad y(t_0) \rightarrow \underbrace{y(t_0 + \Delta t)}_{1}$$

### Split Operators

$$\frac{\partial y}{\partial t} = (\hat{A}y) \qquad y(t_0) = y_0 \qquad t_0 \rightarrow t_0 + \frac{\Delta t}{2} \qquad y^*$$

$$\frac{\partial y}{\partial t} = (\hat{B}y) \qquad y(t_0) = y^* \qquad t_0 \rightarrow t_0 + \Delta t \qquad y^{**}$$

$$\frac{\partial y}{\partial t} = (\hat{A}y) \qquad y\left(t_0 + \frac{\Delta t}{2}\right) = y^{**} \qquad \left(t_0 + \frac{\Delta t}{2}\right) \rightarrow t_0 + \Delta t \qquad \underbrace{y(t_0 + \Delta t)}_{2}$$ Error $O((\Delta t)^2)$

Are 1 and 2 the same? No. They are not the same. Operator splitting introduces error.
Why do we do this? In a reacting flow problem, maybe the two parts have solution methods that are tailored for each part.

### Generalization

$$\frac{\partial y_n(x_i)}{\partial t} = \left(\hat{\mathrm{T}}\,\underline{y}(\underline{x}_i, t)\right) + \left(\hat{S}\,\underline{y}(\underline{x}_i, t)\right)$$

The first term on the right hand side is spatially non-local, usually not that stiff. The stiffness in the first term comes from the use of a fine mesh. The second term on the right hand side is spatially local and stiff; it depends on all species.

Most splitting methods give error O(Δt). Strang splitting is better, because it has an error $O((J(\Delta t))^2)$. So, we say Strang splitting is time accurate. The error is difficult to bound. Usually one runs the solution with a different Δt.

Definition of $\hat{A}$ and $\hat{B}$ : $N_{mesh} \times N_{species}$ number of y's.

Direct coupled: Number of variables scales as $O\left(N_{mesh}^2 N_{sp}^2\right)$. This leads to a storage problem.

$$\frac{\partial y}{\partial t} = \hat{S} y$$

$N_{species}$ at local point. $J \sim N_{sp}^2$. The number of variables scales as $O\left(N_{mesh} N_{sp}^2\right)$ .
Can then solve each mesh point in parallel.

## *Steady State Considerations and Time March*

If you only care about steady state, $\underline{F}\left(\underline{y}\right) = \underline{0}$, the usual approach is to use a Newton-type solver. $\underline{\underline{J}} \Delta \underline{y} = -F\left(y^{guess}\right)$ At $t \to \infty$, Implicit Euler gives the same result.

With a reacting flow, a good guess is difficult. Possible approaches are:

- Work on finding a good guess.
- Solve a simpler problem; then, change the problem gradually into the one you have.
- Time march to steady state (see below); this works for continuous stirred tank reactors (CSTRs).

  $\frac{\partial \underline{y}}{\partial t} = \underline{F}\left(\underline{y}\right)$ $\qquad \underline{y}(t_0) = y_0 \qquad t \to \infty$ $\qquad$ One may have to march for a while.

  $y\left(t_{large}\right) \to y^{guess}$ At large t, the solution may approach a value that can be used as the initial guess for Newton's method.

In biology, there are often multiple steady states, so the solution might jump from one state to another.

In laminar flow, one can analyze the steady states.

In turbulent flow, one can calculate time average values but not fluctuations.

Finding steady state can be difficult: if the problem has more than 10 variables, use *time march*.

## Explicit Euler

Recall that Explicit Euler is numerically unstable.

$$y(t + \Delta t) = y(t) + F(y(t))\Delta t$$

$$y^{new} = y^{old} + F\left(y^{old}\right)\Delta t$$

## Time Marching With Implicit Euler

Although Implicit Euler is not time accurate, it is unconditionally numerically stable.

$$y(t+\Delta t) = y(t) + F\left(y(t+\Delta t)\right)\Delta t$$

$$y^{new} = y^{old} + F\left(y^{new}\right)\Delta t$$

$$\mathrm{F} = y^{new} - y^{old} - F\left(y^{new}\right)\Delta t$$

$$\mathrm{J}_{\mathrm{mn}} = \frac{\partial F_m}{\partial y_n^{new}}\Bigg|_{\underbrace{y^{guess2}}_{\substack{solves\\implicit\\Euler}}} = \delta_{mn} - J\left(y^{guess2}\right)\Delta t$$

$$\underline{\underline{\mathrm{J}}}_{\mathrm{mn}}\Delta y^{refined} = -\mathrm{F}\left(y^{guess2}\right)$$

$$\left(\underline{\underline{I}} - \Delta t\underline{\underline{J}}\right)\Delta y^{refined} = -\Delta y^{guess2} + F\left(y^{guess2}\right)\Delta t$$

Right hand side is close to zero: $\Delta t\left(F - \frac{\Delta y}{\Delta t}\right)$

For small Δt, $\underline{\underline{I}} - \Delta t\underline{\underline{J}} \approx \underline{\underline{I}}$, which is well-conditioned.

Time march with implicit Euler instead of Newton's method. Implicit Euler allows large time steps.