Numerics: Flames are usually solved using Operator Splitting

- Many Equations of form

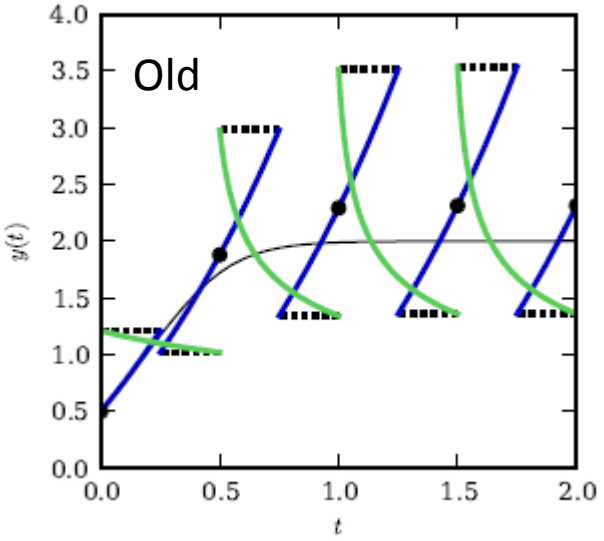
  $$\partial Y_n/\partial t = \text{Reaction}_n(Y) + \text{Transport}_n[Y]$$

- Typical $Y_n(x,y,z,t)$ represent mass fraction of *n*th species. 100 species at 10,000 mesh points = 10^6 state variables.
- Seldom possible to provide good enough initial guess for steady-state, and hard to solve Newton steps with $>10^6$ unknowns, so usually time-march to steady-state.
  - Time-marching can be very slow if you need small Δt!
- Reaction term is local and very stiff. Transport involves gradients (nonlocal after discretization).
- Usually Chemistry Split from Transport
  - Chemistry solved in parallel using stiff ODE solver (e.g. DSL48S)
  - Transport solved using specialized PDE techniques

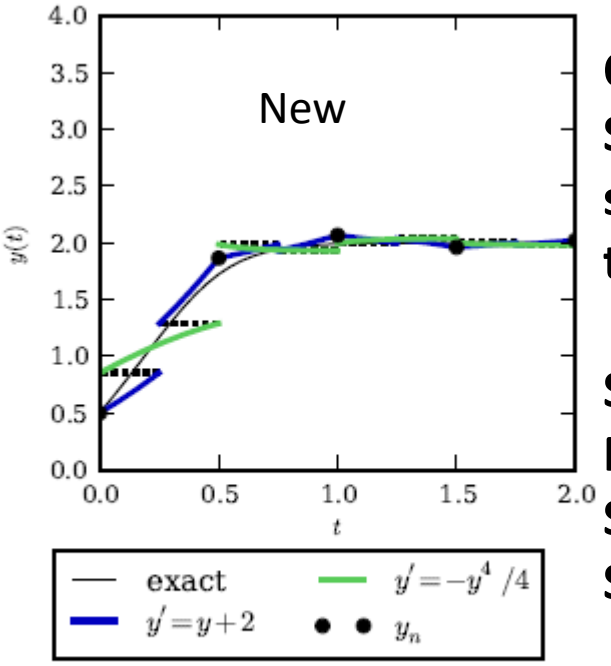
Operator Splitting Methods

- Suppose dy/dt = R + T
- Simplest: first integrate dy/dt=T, then start from $y(t_f)$ and integrate dy/dt=R. Not very accurate.
- Strang: half-step of T, full step R, half step T
  - Second-order accurate, stable.
  - Can be slow to converge to steady-state solution.
- Balanced: dy/dt = (R+c) + (T-c) how to choose c? "Simple Balanced": $c=1/2\ (R(y_n)-T(y_n))$
- "Rebalanced": use averages of R and T over their steps to get a higher-order implicit formula.
  - more accurate and more stable.
  - see Speth et al. SIAM J. Numer. Anal. (2013)

Split each timestep into 3 substeps



Conventional (Strang) Splitting applied to a toy problem. Poor behavior near steady state.



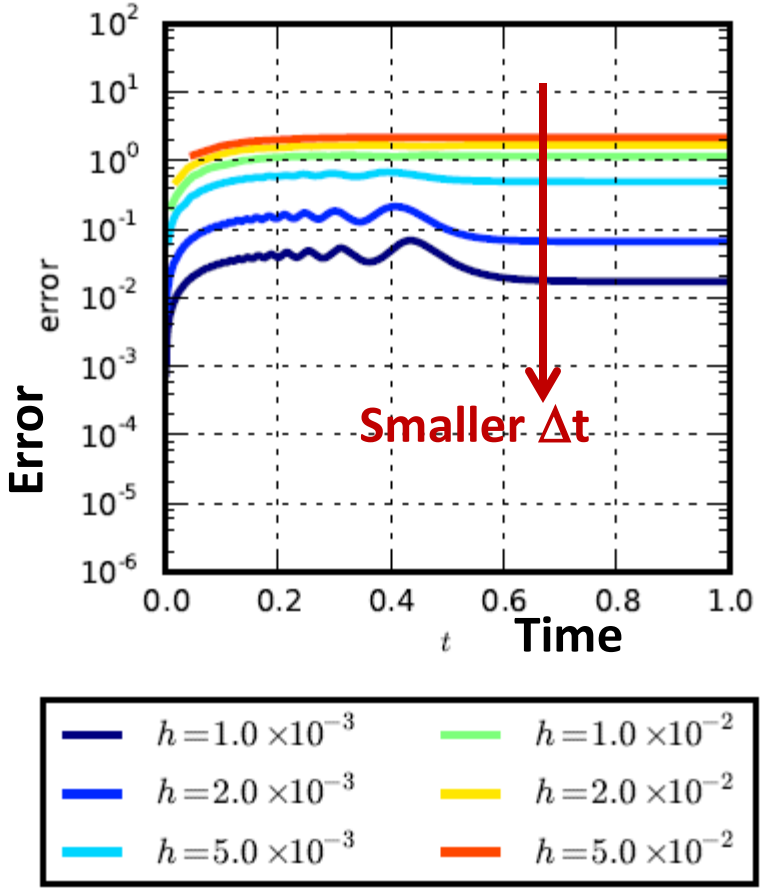
(a) *Simple Balanced Splitting*, $h = 0.5$

Our new Balanced Splitting method stays closer to true trajectory.

Speth, Green, MacNamara & Strang SINUM

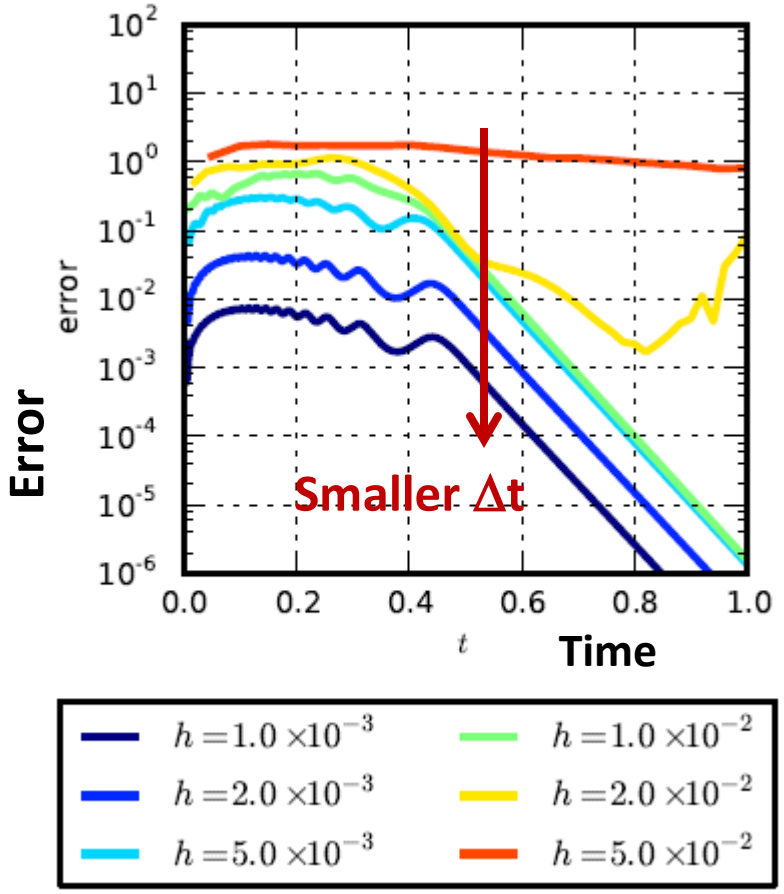
Near Steady State, dY/dt = (Reaction) + (Transport) ~ 0
But each term separately is large. Splitting them makes you walk away from true trajectory during substeps.
Balanced Splitting drastically reduces this walk-away.

Balanced Splitting's Error Exponentially Goes to Zero as Flame steadies out



Strang Splitting:

Constant Splitting Error



Rebalanced Splitting:

Error Vanishes at steady-state

10.34 Numerical Methods Applied to Chemical Engineering

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