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IMEX Lagrangian Methods

2015 Coupled Problems

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Governing Equations

We have a Kinematics equation defining flow of the domain, and time evolution PDE of fields on that same domain

$$\dot{x} - \vec{v} = 0$$

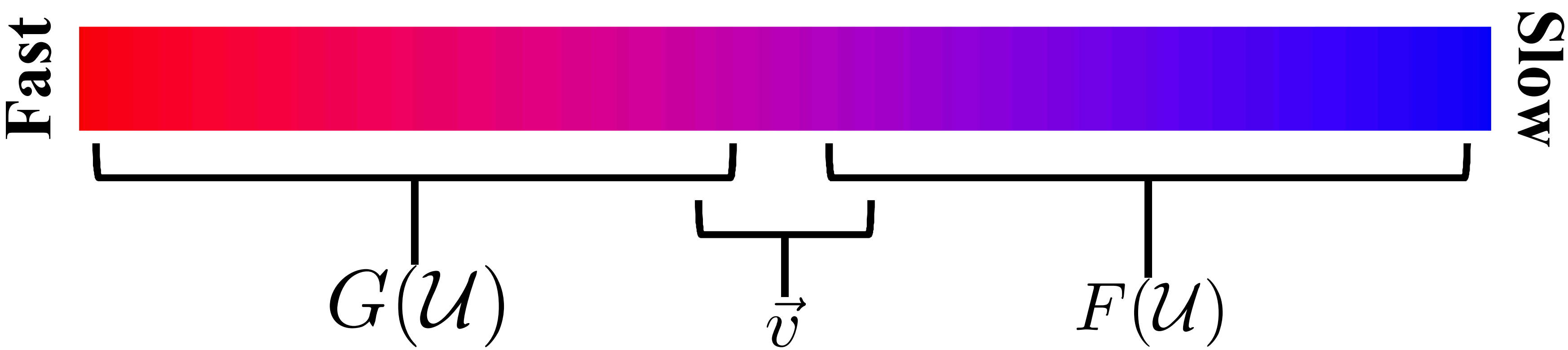
$$\left[\frac{\partial}{\partial t} + \vec{v} \cdot \nabla\right] \mathcal{U} + F(\mathcal{U}) + G(\mathcal{U}) = 0$$

Time scales for the model

This set of equations can be governed by a number of timescales. *Fast* and *slow* are relative terms:

$$\dot{x} - \vec{v} = 0$$

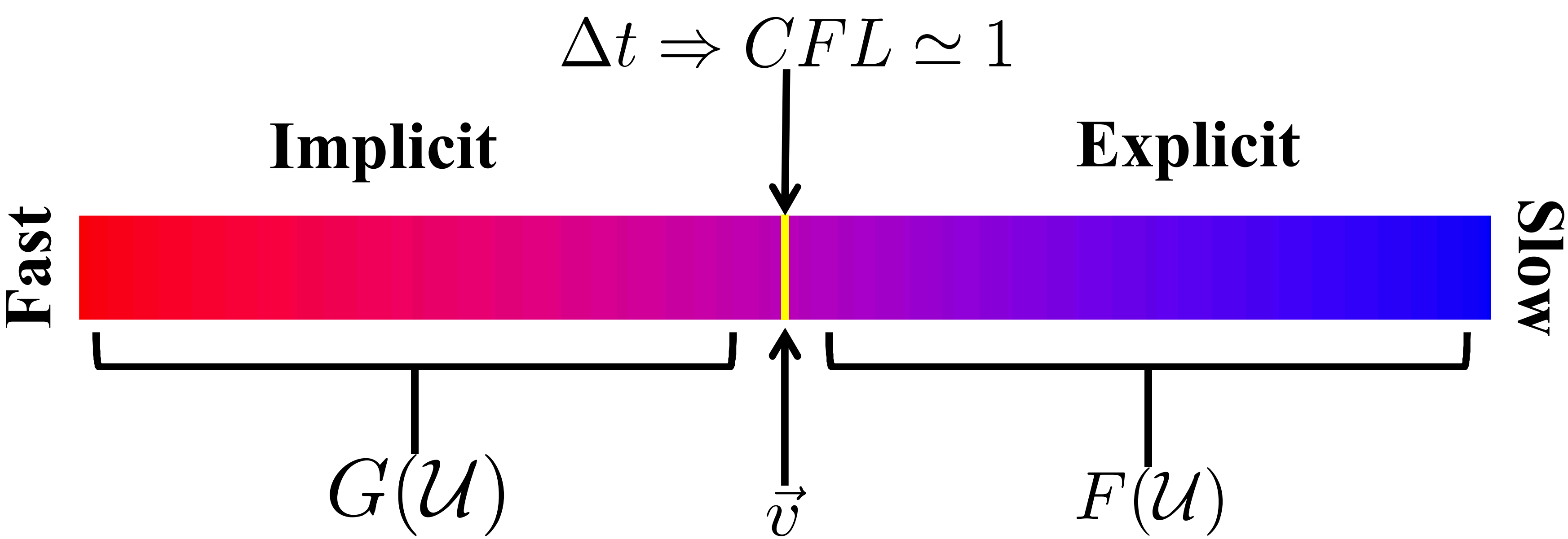
$$\left[\frac{\partial}{\partial t} + \vec{v} \cdot \nabla\right] \mathcal{U} + F(\mathcal{U}) + G(\mathcal{U}) = 0$$



Numerical Time Integration and Time Scales

What time scales are "stiff"?

- Anything "faster than the current time step" must be handled implicitly for stability

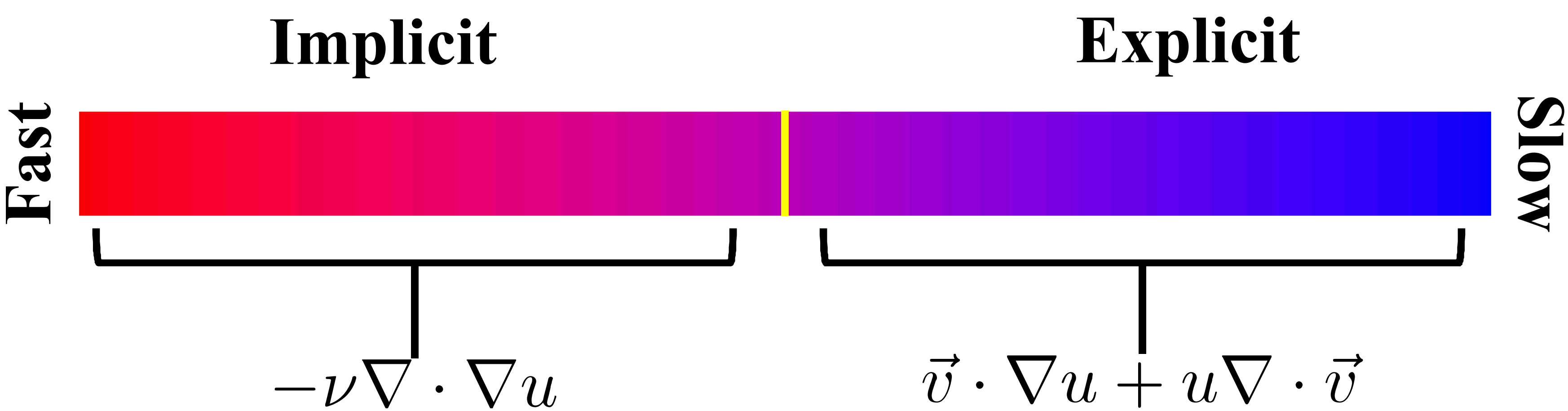


An Example Scalar Case

Assuming that we are following the convected time scale (i.e. $\|\vec{v}\|\Delta t/\Delta x \simeq 1$)

$$\dot{x} - \vec{v} = 0$$

$$\left[\frac{\partial}{\partial t} + \vec{v}\cdot\nabla\right] u + u\nabla\cdot v - \nu\nabla\cdot\nabla u = 0$$



Implicit-Explicit Runge Kutta Methods

Define an ODE where “F” is slow and “G” is fast:

$$\dot{\mathcal{U}} + F(\mathcal{U}) + G(\mathcal{U}) = 0$$

- Implicit-Explicit (IMEX) methods evolve “F” explicitly and “G” implicitly
- There are multi-step (BDF) and multi-stage (RK) versions of these methods
- Our focus is on IMEX-Runge Kutta (IMEX-RK) methods

IMEX-RK Methods

We start with on ODE:

$$\dot{\mathcal{U}} + F(\mathcal{U}) + G(\mathcal{U}) = 0$$

- Two Butcher tableau's are used:

$\begin{array}{c|c} c & A \\ \hline & b^t \end{array}$ is for implicit terms, $\begin{array}{c|c} \hat{c} & \hat{A} \\ \hline & \hat{b}^t \end{array}$ is for explicit terms

- An s-stage IMEX-RK method satisfies ('c' defines time node)

$$\mathcal{U}^{(i)} = \mathcal{U}^n - \Delta t \sum_{j=1}^{i-1} \hat{A}_{ij} F(\mathcal{U}^{(j)}) - \Delta t \sum_{j=1}^{i} A_{ij} G(\mathcal{U}^{(j)}) \qquad \text{for } i = 1 \ldots s,$$

$$\mathcal{U}^{n+1} = \mathcal{U}^n - \Delta t \sum_{i=1}^{s} \hat{b}_i F(\mathcal{U}^{(i)}) - \Delta t \sum_{i=1}^{s} b_i G(\mathcal{U}^{(i)})$$

IMEX-RK Methods

Written as an algorithm, the previous expressions result in:

for $i = 1 \dots s$ **do**

$\tilde{\mathcal{U}} \leftarrow \mathcal{U}^n - \Delta t \sum_{j=1}^{i-1} \hat{A}_{ij} f_j - \Delta t \sum_{j=1}^{i-1} A_{ij} g_i$

Solve $\mathcal{U}^{(i)} - \tilde{\mathcal{U}} + \Delta t A_{ii} G(\mathcal{U}^{(i)}) = 0$ for $\mathcal{U}^{(i)}$

$f_i \leftarrow F(\mathcal{U}^{(i)})$

$g_i \leftarrow (\tilde{\mathcal{U}} - \mathcal{U}^{(i)}) \frac{1}{A_{ii} \Delta t}$

end for

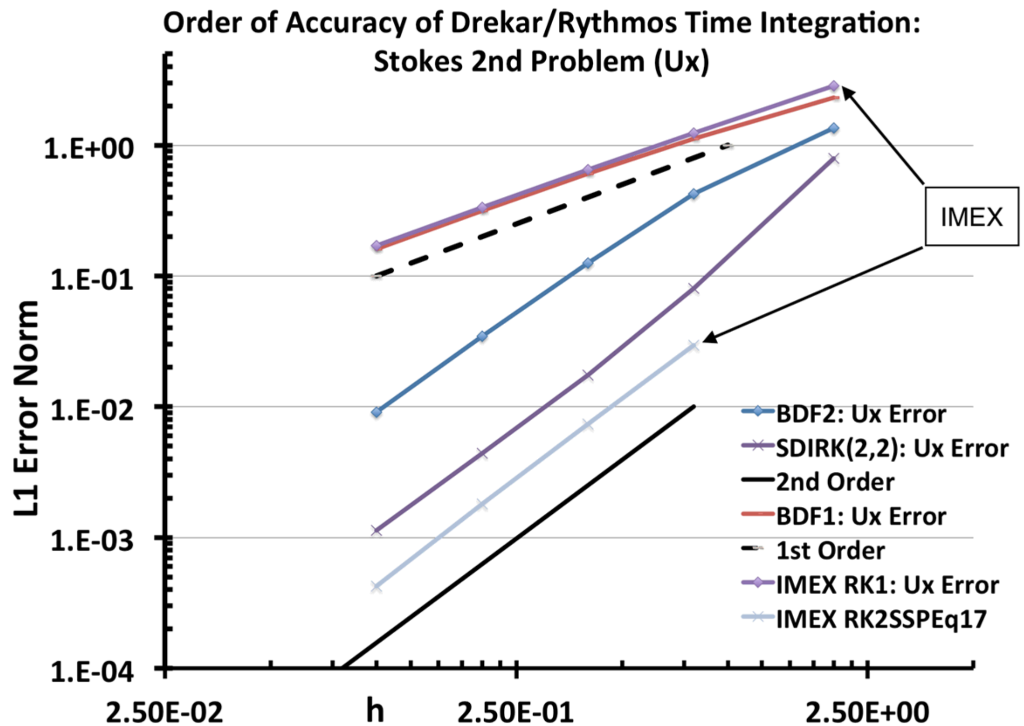
$\mathcal{U}^{n+1} \leftarrow \mathcal{U}^n - \Delta t \sum_{i=1}^{s} \hat{b}_i f_i - \Delta t \sum_{i=1}^{s} b_i g_i$

(Note: For i=1, $\tilde{U}=U^n$)

An Eulerian IMEX Example: Stokes 2nd Problem

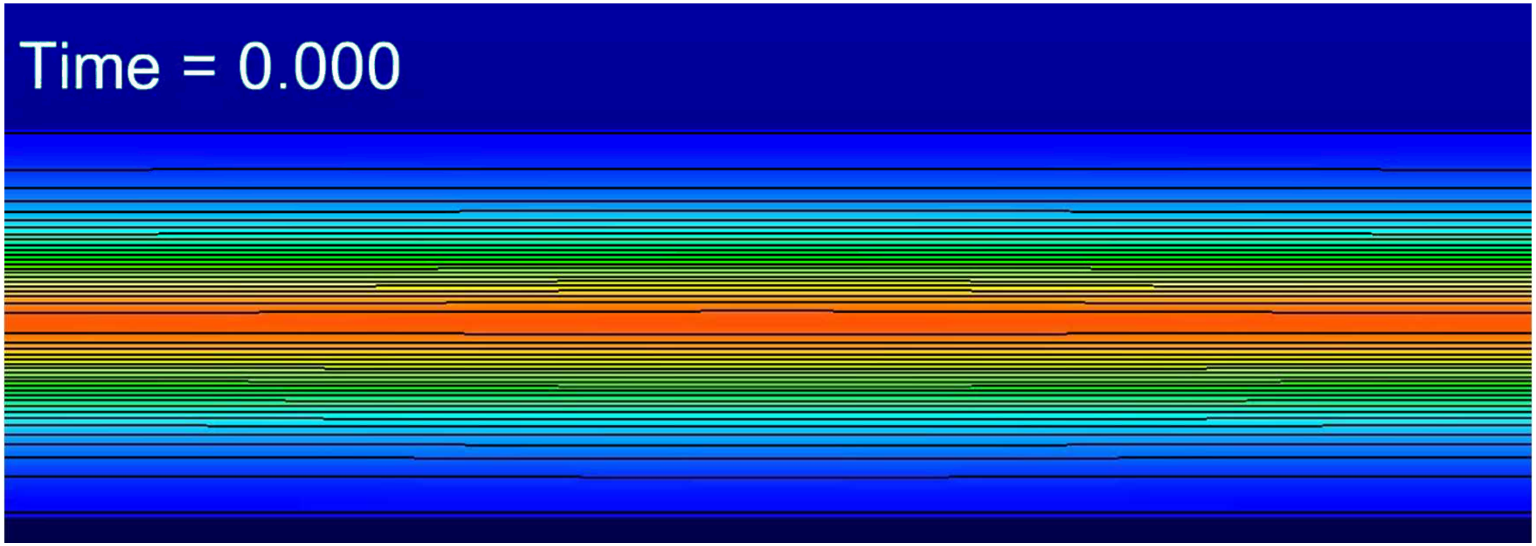
Convergence in time for Stokes 2nd Problem

- Low-mach CFD
- Run at fixed CFL
- Explicit advection
- Implicit diffusion and sound speed



Take Home: IMEX methods in Eulerian frame achieve expected order of accuracy

2D Tearing Mode: Low Mach ($M \sim 10^{-4}$) compressible MHD



<u>Approx. Computational Time Scales:</u>

- Divergence Constraint ($\nabla \cdot \mathbf{B} = 0$): $1/\infty = 0$
- Fast Magnetosonic Wave (c_f): 10^{-4} to 10^{-2}
- Alfven Wave (c_a): 10^{-4} to 10^{-2}
- Slow Magnetosonic Wave (c_s): 10^{-2} to 10^{-1}
- Sound Wave (c): 10^{-2}
- Advection(c_v): ∞ to 10^{1}
- Diffusion: 10^{-4} to 10^{-2}
- Macroscopic Tearing Mode: 10^{2}

<u>Wave speeds</u>

$$\|\mathbf{u}\|, \|\mathbf{u}\| \pm c_s, \|\mathbf{u}\| \pm c_a, \|\mathbf{u}\| \pm c_f, \pm c_h$$

Take Home: IMEX can handle multiple timescales

IMEX SSP3 (3,2,2) 2nd order
Max CFLs:

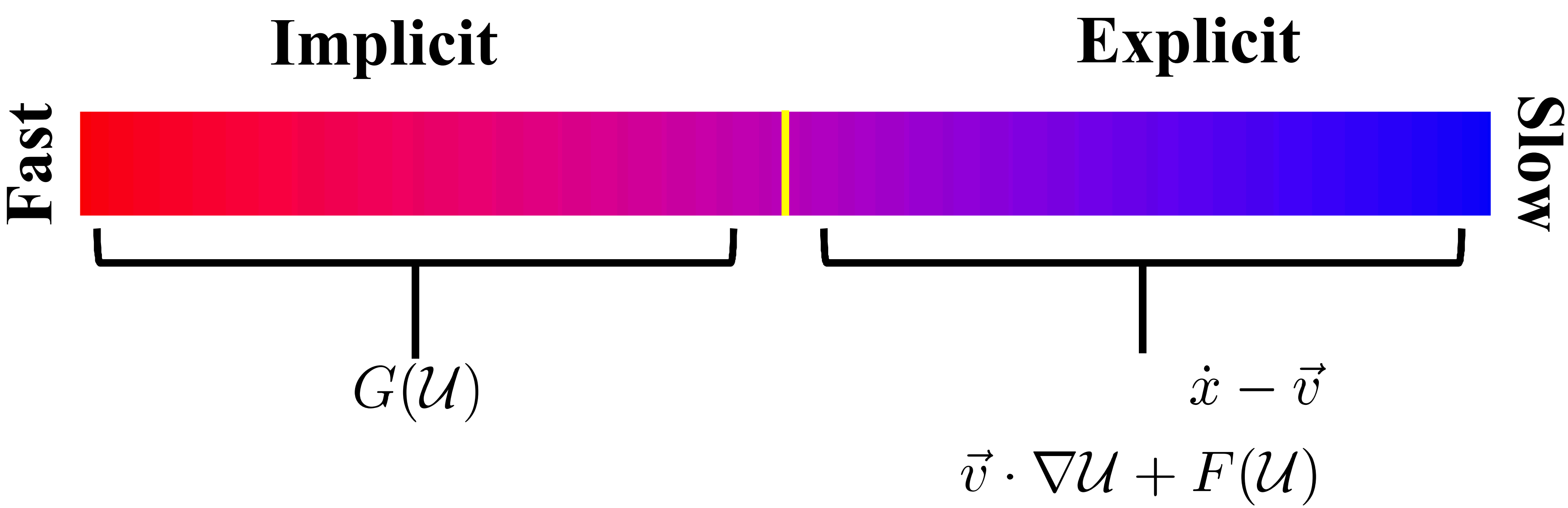
$CFL_{div} = \infty$
$CFL_{cf} \sim 10^4$ to 10^3
$CFL_{cA} \sim 10^4$ to 10^3
$CFL_{cs} \sim 10^2$ to 10^1
$CFL_{c} \sim 10^2$ to 10^1
$CFL_{cv} \sim 0.33$

Lagrangian Formulation

We assume that kinematics will be treated explicitly (there may be a faster mode to resolve explicitly):

$$\dot{x} - \vec{v} = 0$$

$$\left[\frac{\partial}{\partial t} + \vec{v} \cdot \nabla\right] \mathcal{U} + F(\mathcal{U}) + G(\mathcal{U}) = 0$$



Lagrangian Formulation: Semi-Discrete Form

Replacing material time derivative with total time derivative in Lagrangian frame and discretizing in space gives:

$$\dot{x} - \vec{v}(x, \mathcal{U}) = 0$$

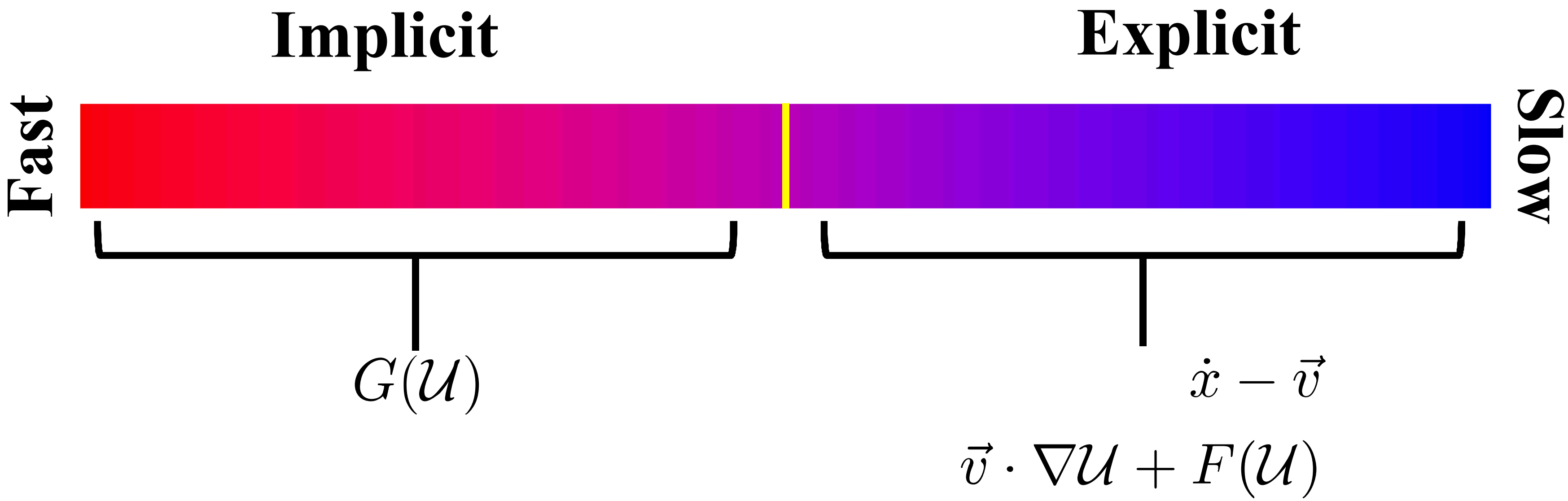
$$M(x)\frac{d\mathcal{U}}{dt} + F_h(x, \mathcal{U}) + G_h(x, \mathcal{U}) = 0$$

Writing this in an ODE form appropriate for applying IMEX-RK gives:

$$\dot{x} - \vec{v}(x, \mathcal{U}) = 0$$

$$\frac{d\mathcal{U}}{dt} + M(x)^{-1}F_h(x, \mathcal{U}) + M(x)^{-1}G_h(x, \mathcal{U}) = 0$$

IMEX Formulation



$$x^{(i)} = x^n - \Delta t \sum_{j=1}^{i-1} \hat{A}_{ij} \vec{v}(x^{(j)}, \mathcal{U}^{(j)}) \qquad \text{for } i = 1 \ldots s,$$

$$\mathcal{U}^{(i)} = \mathcal{U}^n - \Delta t \sum_{j=1}^{i-1} \hat{A}_{ij} M^{-1}(x^{(j)}) F_h(x^{(j)}, \mathcal{U}^{(j)}) - \Delta t \sum_{j=1}^{i} A_{ij} M^{-1}(x^{(j)}) G_h(x^{(j)}, \mathcal{U}^{(j)}) \qquad \text{for } i = 1 \ldots s,$$

$$x^{n+1} = x^n - \Delta t \sum_{i=1}^{s} \hat{b}_i \vec{v}(x^{(i)}, \mathcal{U}^{(i)})$$

$$\mathcal{U}^{n+1} = \mathcal{U}^n - \Delta t \sum_{i=1}^{s} \hat{b}_i M^{-1}(x^{(i)}) F_h(x^{(i)}, \mathcal{U}^{(i)}) - \Delta t \sum_{i=1}^{s} b_i M^{-1}(x^{(i)}) G_h(x^{(i)}, \mathcal{U}^{(i)})$$

IMEX Formulation: Algorithm

Coordinates are evolved explicitly in time, remaining terms are evolved implicitly. This is a partitioned IMEX scheme. Only one mass inversion per stage is required.

for $i = 1 \ldots s$ **do**

$x^{(i)} \leftarrow x^n - \Delta t \sum_{j=1}^{i-1} \hat{A}_{ij} v_j$

$\tilde{\mathcal{U}} \leftarrow \mathcal{U}^n - \Delta t \sum_{j=1}^{i-1} \hat{A}_{ij} f_j - \Delta t \sum_{j=1}^{i-1} A_{ij} g_i$

Solve $M(x^{(i)}) \left(\mathcal{U}^{(i)} - \tilde{\mathcal{U}} \right) + \Delta t A_{ii}(x^{(i)}) G_h(x^{(i)}, \mathcal{U}^{(i)}) = 0$ for $\mathcal{U}^{(i)}$

$v_i \leftarrow \vec{v}(x^{(i)}, \mathcal{U}^{(i)})$

$f_i \leftarrow M^{-1}(x^{(i)}) F_h(x^{(i)}, \mathcal{U}^{(i)})$

$g_i \leftarrow (\tilde{\mathcal{U}} - \mathcal{U}^{(i)}) \frac{1}{A_{ii} \Delta t}$

end for

$x^{n+1} \leftarrow x^n - \Delta t \sum_{1=1}^{s} \hat{b}_i v_i$

$\mathcal{U}^{n+1} \leftarrow \mathcal{U}^n - \Delta t \sum_{i=1}^{s} \hat{b}_i f_i - \Delta t \sum_{i=1}^{s} b_i g_i$

IMEX-RK Tableaus

Name	*Order*	*Implicit Tab.*	*Explicit Tab.*
First Order	1st	$\begin{array}{c\|cc} 0 & 0 & 0 \\ 1 & 0 & 1 \\ \hline & 0 & 1 \end{array}$	$\begin{array}{c\|cc} 0 & 0 & 0 \\ 1 & 1 & 0 \\ \hline & 1 & 0 \end{array}$
SSP2	2nd	$\begin{array}{c\|cc} \gamma & \gamma & 0 \\ 1-\gamma & 1-2\gamma & \gamma \\ \hline & 1/2 & 1/2 \end{array}$ $\gamma = 1 - 1/\sqrt{2}$	$\begin{array}{c\|cc} 0 & 0 & 0 \\ 1 & 1 & 0 \\ \hline & 1/2 & 1/2 \end{array}$
ARS 2-3-3	3rd	$\begin{array}{c\|ccc} 0 & 0 & 0 & 0 \\ \gamma & 0 & \gamma & 0 \\ 1-\gamma & 0 & 1-2\gamma & \gamma \\ \hline & 0 & 1/2 & 1/2 \end{array}$ $\gamma = (3+\sqrt{3})/6$	$\begin{array}{c\|ccc} 0 & 0 & 0 & 0 \\ \gamma & \gamma & 0 & 0 \\ 1-\gamma & \gamma-1 & 2-2\gamma & 0 \\ \hline & 0 & 1/2 & 1/2 \end{array}$ $\gamma = (3+\sqrt{3})/6$

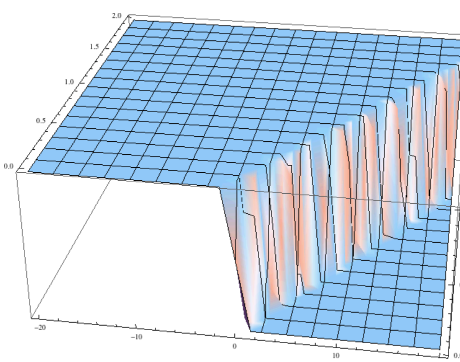
Example: Thermal Wave Problem

Example transient convection-diffusion-reaction multiphysics problems with exact solutions.

Traveling wave: Translating constant velocity of $\dfrac{U}{\delta}$

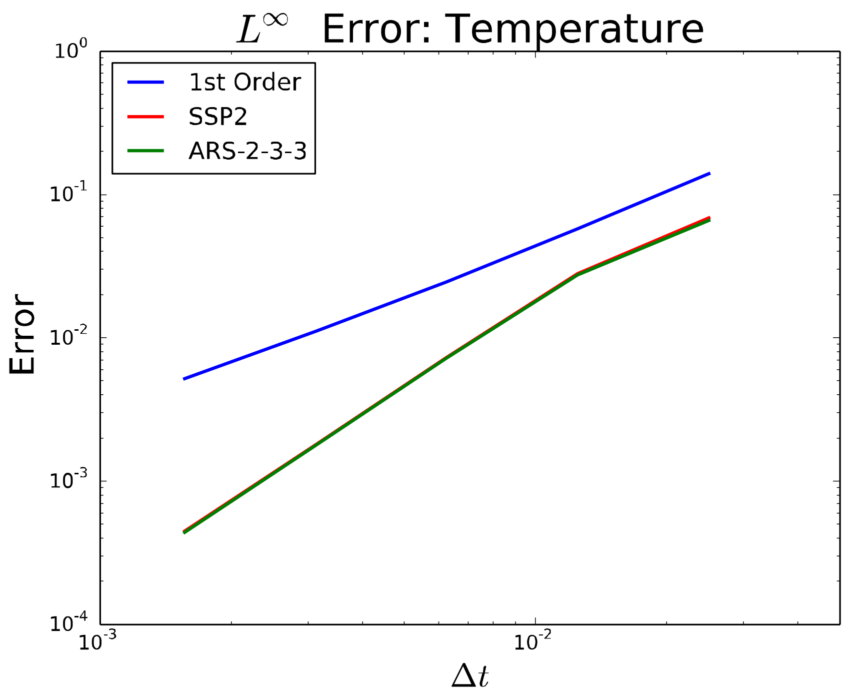
Convection-diffusion-reaction equation and solution:

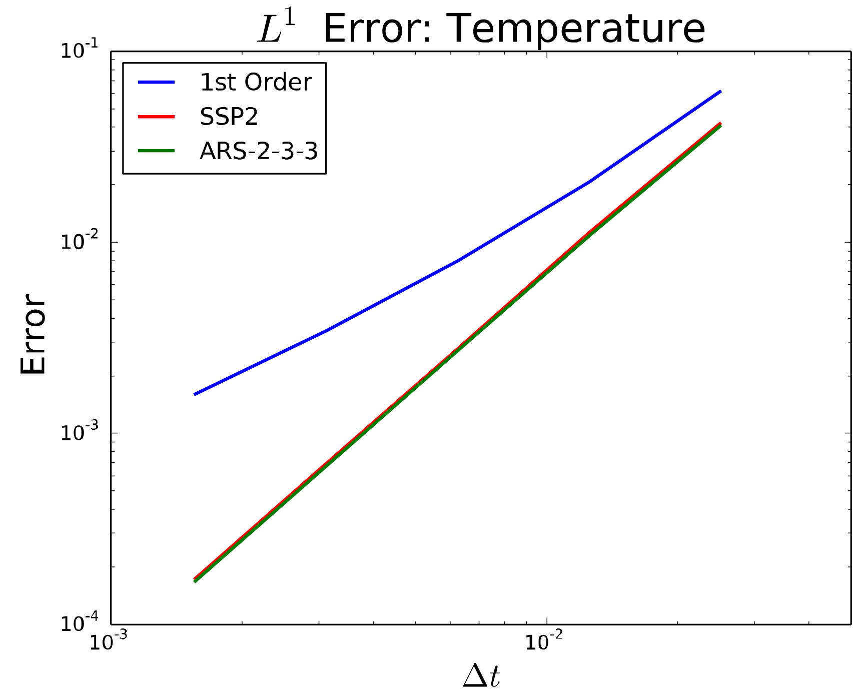
$$\frac{\partial T}{\partial t} + \frac{\partial}{\partial x}\left(\frac{U}{\delta}T - \lambda\frac{\partial T}{\partial x}\right) - \frac{8\lambda}{\delta^2}T^2(1-T) = 0$$



$$T(x,t) = \frac{1}{2}\left(1.0 - tanh\left[\frac{x-(2\lambda+U)t/\delta}{\delta}\right]\right)$$

Thermal Wave Results





Using a 1D finite difference on a domain of [-5,5] for 0.5s:

- Model parameters: U=1.0, λ=0.1, δ=0.2
- Run with fixed CFL (Δt/Δx=1)…best convergence rate is $O(\Delta t^2)$
- Coordinate value is "exact" (constant advection)

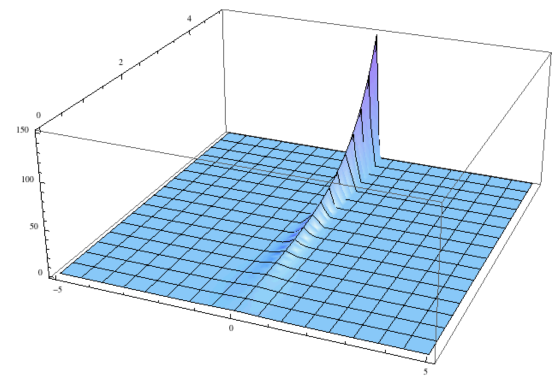
Example: Compression

Example convection-diffusion-reaction equation with a compression velocity: $u = -U \ tanh\left[\frac{x}{\delta}\right]$

Equation and solution:

$$\frac{\partial e}{\partial t} + \frac{\partial}{\partial x}\left(ue - \lambda\frac{\partial e}{\partial x}\right) + S_e = 0$$

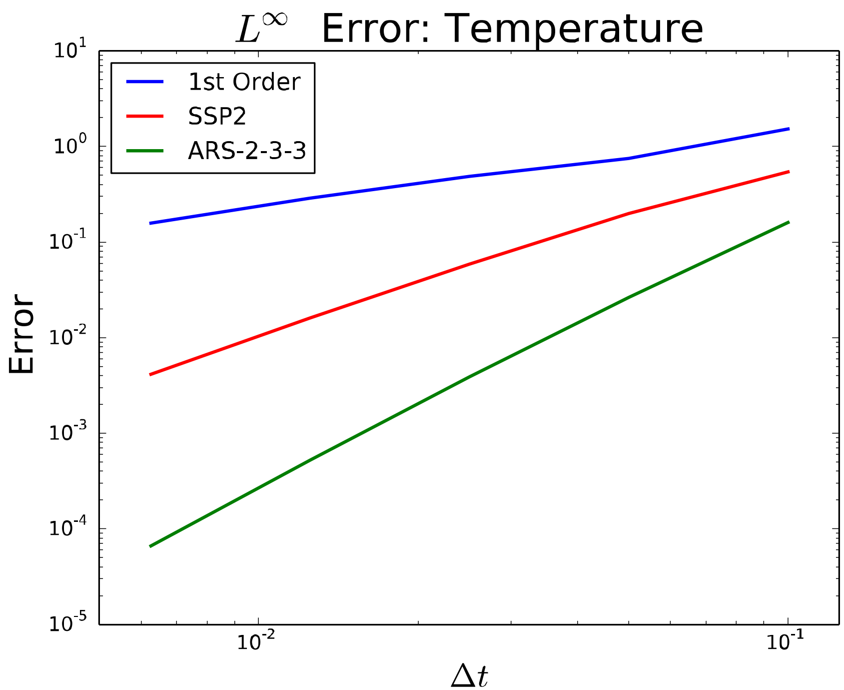
$$e = \left(1.0 + exp(t/\tau)\ sech\left[\frac{(1.0+t^2)x}{\delta}\right]\right)$$

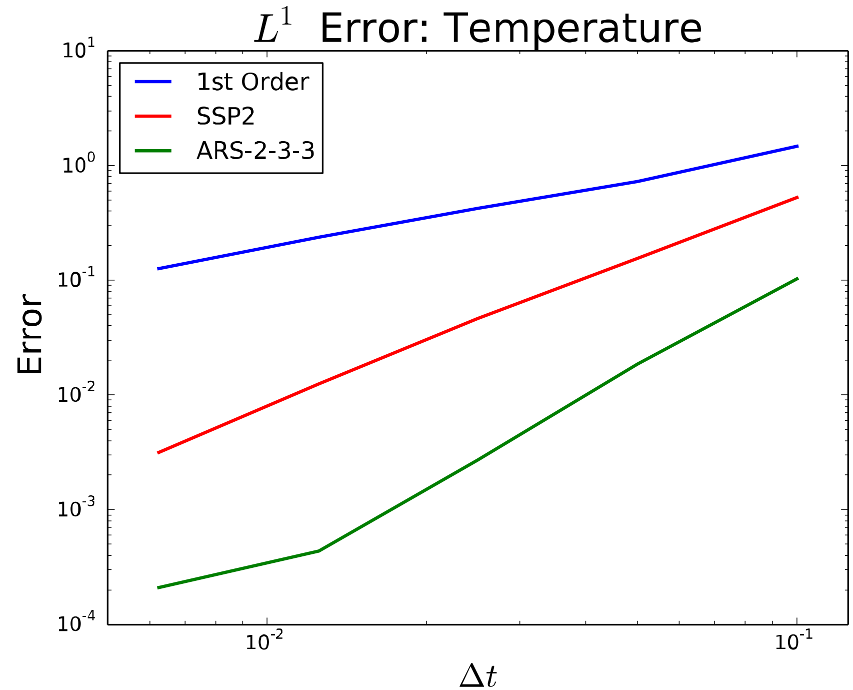


Nonlinear Source term:

$$f_1 = \delta\ \tau\ U(1.0 - (u/U)^2)$$
$$f_2 = -(1.0+t^2)^2\ \lambda\ \tau + \delta^2 - f1$$
$$f_3 = \tau\ \delta\ (2\ t\ x + (1.0+t^2)\ u)\ tanh\left[\frac{((1.0+t^2)x}{\delta}\right]$$
$$S_e = \frac{\left[f_1 + (1.0-e) * \left(f_2 + \ 2\ \lambda\ \tau(1.0+t^2)^2\ [exp(-t/\tau)]^2(1.0-e)^2 - f_3\right)\right]}{\delta^2\ \tau}$$

Compression Results

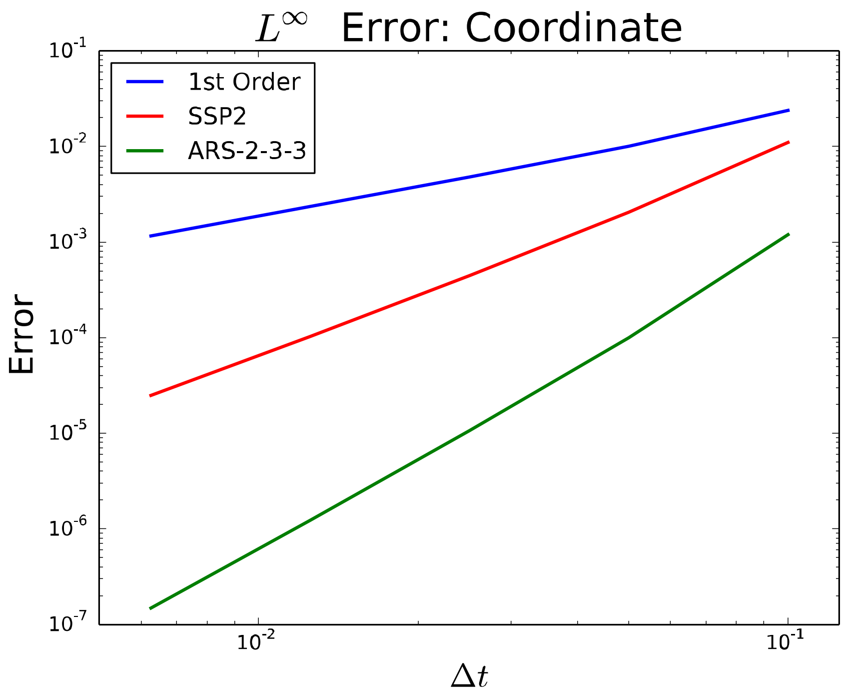


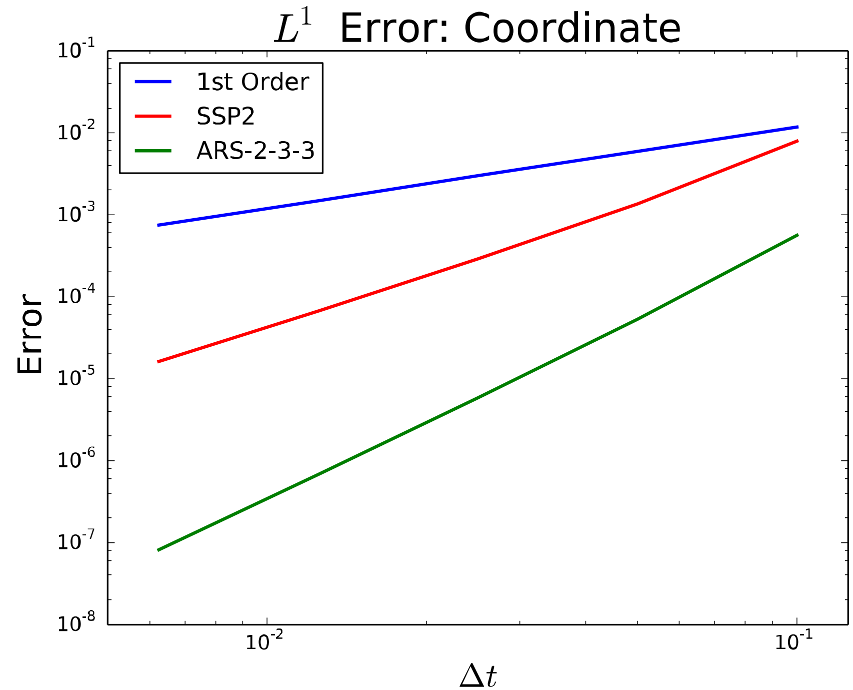


Using a 1D finite difference on a domain of [-5,5] for 0.5s:

- Model parameters: U=1.0, $\lambda=10^{-4}$, δ=0.1, τ=1.0
- Run with fixed mesh (Δx=10.0/1021)

Compression Results





Using a 1D finite difference on a domain of [-5,5] for 0.5s:

- Model parameters: U=1.0, $\lambda=10^{-4}$, $\delta=0.1$, $\tau=1.0$
- Run with fixed mesh ($\Delta x=10.0/1021$)

Summary

Discussed IMEX methods in Eulerian frame

- Provides a well structured mechanism for separation of time scales into slow (explicit) and fast (implicit)
- IMEX Runge-Kutta methods have 2 Butcher tableaus
- Showed convergence of for CFD example and multiple timescale capabilities for MHD tearing mode problem

Developed IMEX Lagrangian formulation

- Required handling of mass matrix and using a partitioned IMEX-RK scheme for explicit kinematics
- Showed convergence results of up to 3rd order for example finite difference problems