Implicit-explicit Runge Kutta schemes for convection-degenerate diffusion PDE

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- This talk is based on work with:
  - Sebastiano Boscarino (U. Catania),
  - Raimund Bürger (U. Concepción)
  - Rosa Donat (U. Valencia)
  - Francisco Guerrero (U. Valencia)
  - Daniel Inzunza (U. Concepción)
  - Giovanni Russo (U. Catania)
  - Luis Miguel Villada (U. Bio Bio).

  and is intended to be an exposition of my recent experience in the field:
  - **R. Bürger, P. M., and L. M. Villada**. *SIAM J. Sci. Comp.*, 2013.
  - **S. Boscarino, R. Bürger, P. M., G. Russo, and L. M. Villada**. *SIAM J. Sci. Comp.*, 2015.
  - **R. Donat, F. Guerrero, and P. M.** *Appl. Numer. Math.*, 2018.
  - **R. Bürger, D. Inzunza, P. M., and L. Villada**. *Numer. Meth. PDE*, 2019.
  - **R. Bürger, D. Inzunza, P. M., and L. Villada**. to appear in *Appl. Numer. Math.*, 2019.

Outline

1. Convective PDE with degenerate diffusion
2. Implicit-Explicit Runge-Kutta schemes for diffusive kinematic flow models
   - Nonlinearly implicit-explicit schemes
   - Diffusively corrected multi-species kinematic flow models
   - Numerical experiments with Nonlinearly IMEX schemes
   - Linearly implicit-explicit schemes
   - Numerical experiments with Linearly IMEX schemes
3. IMEX-RK schemes for gradient flow equations
   - Nonlinearly Implicit-Explicit schemes
   - Numerical experiments
4. Conclusions
   - Ongoing and future work

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Convection-diffusion equations and MOL

- **Goal:** efficient numerical solution of convection-diffusion system of m equations with m unknowns

$$u_t + \nabla \cdot \left(f^{\mathsf{c}}[u] - f^{\mathsf{d}}(u, \nabla u) \right) = 0, \quad \nabla \cdot \equiv \text{div} = \text{div}_{\boldsymbol{x}}$$

$$u = u(\boldsymbol{x}, t) \in \mathbb{R}^m, \quad \boldsymbol{x} \equiv \text{space}, \quad t \equiv \text{time}$$

$f^{\mathsf{c}}[u] \equiv$ convective fluxes (may depend non-locally on u)

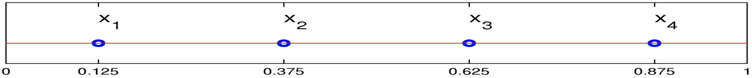
$f^{\mathsf{d}}(u, \nabla u) \equiv$ diffusive fluxes

$$+ B.C. + I.C.$$

- (May be strongly) **Degenerate** diffusion, i.e. f^{d} vanishes for some values of $u \Rightarrow$ discontinuities may appear (**weak solutions**) and **numerical methods should cope with them**.
- Accuracy obtained by **M**ethod **O**f **L**ines (spatial discretization by **finite differences**, finite volumes, Galerkin techniques,...)

Linear convection-diffusion

- $u_t + \gamma u_x - \delta u_{xx} = 0$, $x \in (0,1)$, periodic BC, $\gamma, \delta > 0$
- Consider x_j, $j = 1, \ldots, L$, in equispaced grid ($\Delta x = \frac{1}{L}$), e.g.



- Use F.D. (**upwind for convection**) in $(u_t + \gamma u_x - \delta u_{xx})(x_j, t) = 0 \Rightarrow$

$$u_t(x_j,t) + \gamma \frac{u(x_j,t) - u(x_{j-1},t)}{\Delta x} - \delta \frac{u(x_{j+1},t) - 2u(x_j,t) + u(x_{j-1},t)}{\Delta x^2} \approx 0$$

- Get **spatial semidiscretization** for $\boxed{v_j(t) \approx u(x_j,t)}$

$$\Rightarrow v_j'(t) = \gamma \frac{-v_j(t) + v_{j-1}(t)}{\Delta x} + \delta \frac{v_{j+1}(t) - 2v_j(t) + v_{j-1}(t)}{\Delta x^2}$$

Method of lines: $u_t + \gamma u_x - \delta u_{xx} = 0,\ x \in (0,1)$

- Linear PDE and linear discretization (by F.D.) $\Rightarrow$ linear ODE:

$$\begin{bmatrix} v_1'(t) \\ \vdots \\ v_m'(t) \end{bmatrix} = \frac{\gamma}{\Delta x} \underbrace{\begin{bmatrix} -1 & 0 & \dots & 1 \\ 1 & -1 & \ddots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & \dots & 1 & -1 \end{bmatrix}}_{C} \begin{bmatrix} v_1(t) \\ \vdots \\ v_m(t) \end{bmatrix}$$

$$+ \frac{\delta}{\Delta x^2} \underbrace{\begin{bmatrix} -2 & 1 & 0 & \dots & 1 \\ 1 & -2 & 1 & \ddots & 0 \\ \dots & \dots & \dots & \dots & \dots \\ 1 & \dots & 0 & 1 & -2 \end{bmatrix}}_{D} \begin{bmatrix} v_1(t) \\ \vdots \\ v_m(t) \end{bmatrix}$$

- **Spatial semidiscretization:**

$$v'(t) = Av(t), \quad A = \frac{\gamma}{\Delta x} C + \frac{\delta}{\Delta x^2} D \in \mathbb{R}^{L \times L}, \quad v(t) \in \mathbb{R}^L$$

Fully discrete numerical method

- **Fully discrete scheme** for $v_j^n \approx v_j(t_n) \approx u(x_j, t_n)$ by applying, e.g., **Euler's method** to $v' = Av$ ($\Delta t = t_{n+1} - t_n$ for sake of argument):

$$v^{n+1} = v^n + \Delta t\, Av^n = (I + \Delta t\, A)v^n \Rightarrow$$
$$v^n = (I + \Delta t A)^n v^0, v_j^0 = u(x_j, 0)$$

- Use spectral decomposition of A (with eigenvalues $\lambda_p = \lambda_p(A)$) for

$$(I + \Delta t A)^n v^0 = \sum_p (1 + \Delta t \lambda_p)^n z_p$$

$\Rightarrow$ no blow up (**exact solutions do not**) if $|1 + \Delta t \lambda_p| \leq 1$, $\forall p$

- **von Neumann analysis** yields eigenvalues λ_p, $p = 0, \ldots, m-1$ so that

$$\max_p |\lambda_p| \approx 2\left(\frac{\gamma}{\Delta x} + \frac{2\delta}{\Delta x^2}\right)$$

Stiffness - stability

- Increasing **stiffness** (**large eigenvalues**) when $\Delta x \to 0$ (more from D):

$$\max_p |\lambda_p| \approx 2\left(\frac{\gamma}{\Delta x} + \frac{2\delta}{\Delta x^2}\right) \uparrow \infty$$

- Many tiny time steps Δt to attain fixed $T > 0$ (**no need for accuracy**):

$$|1 + \Delta t \lambda_p| \leq 1, \quad \forall p \iff \Delta t \left(\frac{\gamma}{\Delta x} + \frac{2\delta}{\Delta x^2}\right) \leq 1$$

- No restriction on Δt for stability of e.g. **Implicit Euler's method**, but
  - $\Delta t \propto \Delta x$ for accuracy
  - Need to ensure that $v^{n+1} = v^n + \Delta t A v^{n+1}$ has (uniquely determined) solution $v^{n+1} = (I - \Delta t A)^{-1} v^n$ i.e., $I - \Delta t A$ is invertible (✓ example)
  - **Need to solve the equation to compute it!**

Nonlinear stability

- Nonlinear stability analysis for MOL in **[Verwer and Sanz-Serna (1984)]** is intricate and/or of limited applicability.
- **Poor man's analysis** (mostly unjustified) based on linearization about constant states $\bar{u}$ and linear stability analysis:

$$u_t + f(u)_x - (A(u)u_x)_x = 0 \Rightarrow$$

(**linearization about** $\bar{u}$, $u(x) = \bar{u} + \widetilde{u}(x)$)

$$\widetilde{u}_t + \underbrace{f'(\bar{u})}_{\gamma}\widetilde{u}_x - \underbrace{A(\bar{u})}_{\delta}\widetilde{u}_{xx} = 0 \Rightarrow$$

$$\textbf{stiffness measure} = 2\left(\frac{|\gamma|}{\Delta x} + \frac{2\delta}{\Delta x^2}\right) = 2\left(\frac{|f'(\bar{u})|}{\Delta x} + \frac{2A(\bar{u})}{\Delta x^2}\right)$$

- For systems, it turns into practical bound for Δt, for **semiempirical** K

$$\Delta t\left(\frac{\max_{p,\bar{u}} |\lambda_p(f'(\bar{u}))|}{\Delta x} + \frac{2\max_{p,\bar{u}} \lambda_p(A(\bar{u}))}{\Delta x^2}\right) \leq K$$

Spatial discretization

- In general, the **spatial discretization** of

$$u_t + \nabla \cdot \Big(f^{\mathsf{c}}[u] - f^{\mathsf{d}}(u, \nabla u) \Big) = 0, \text{ is:}$$

$$v' = \mathcal{C}(v) + \mathcal{D}(v) \quad \left(\mathcal{C}(v) = -\frac{\gamma}{\Delta x} C v, \mathcal{D}(v) = \frac{\delta}{\Delta x^2} D v \text{ in example}\right)$$

- To cope with weak solutions, both terms are derived by divided differences of **numerical fluxes** (**Lax-Wendroff theorem**), i.e., in 1D

$$\mathcal{C}(v)_j = -\frac{\widehat{f^{\mathsf{c}}}(v)_{j+\frac{1}{2}} - \widehat{f^{\mathsf{c}}}(v)_{j-\frac{1}{2}}}{\Delta x}, \quad \mathcal{D}(v)_j = \frac{\widehat{f^{\mathsf{d}}}(v)_{j+\frac{1}{2}} - \widehat{f^{\mathsf{d}}}(v)_{j-\frac{1}{2}}}{\Delta x}$$

- Numerical fluxes $\widehat{f^{\mathsf{d}}}(v)_{j+\frac{1}{2}}$ are (relatively) simple, but $\widehat{f^{\mathsf{c}}}(v)_{j+\frac{1}{2}}$ are not: **shock-capturing**, need to take into account **upwind direction** for stability and use highly nonlinear reconstruction (MUSCL, ENO, WENO, $\cdots$) for **nonoscillatory accuracy**.

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Implicit-Explicit schemes

- Implicit methods are attractive for not restricting Δt.
- But, when nonlinearity comes in (either from PDE or spatial discretization or both), applying an implicit solver to

$$v' = \mathcal{C}(v) + \mathcal{D}(v)$$

e.g., Implicit Euler's method

$$v^{n+1} = v^n + \Delta t(\mathcal{C}(v^{n+1}) + \mathcal{D}(v^{n+1})),$$

requires solving nonlinear systems (by e.g. Newton's method).
- Dealing with the nonlinearity (**nonlinear solver implementation, existence and uniqueness of solutions**) for $\mathcal{D}$ is relatively easy, but it is not so for $\mathcal{C}$.
- We aim to use Implicit-Explicit schemes **[Crouzeix (1980)]**, as

$$v^{n+1} = v^n + \Delta t(\mathcal{C}(v^n) + \mathcal{D}(v^{n+1})),$$

but with higher-order accuracy.

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Nonlinearly implicit-explicit schemes

- **[Ascher, Ruuth, and Spiteri (1997)]** apply **P**artitioned **R**unge-**K**utta method

defined by $\begin{array}{c|c} \widetilde{c} & \widetilde{A} \\ \hline & \widetilde{b}^T \end{array}$, $\widetilde{a}_{i,j} = 0, j \geq i,$ $\begin{array}{c|c} c & A \\ \hline & b^T \end{array}, a_{i,j} = 0, j > i$

ERK **DIRK**

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1 & 0 \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

Heun

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & \frac{1}{2} & \frac{1}{2} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

Crank-Nicolson

to the **split** system (which is equivalent to $v' = \mathcal{C}(v) + \mathcal{D}(v)$)

$$\begin{cases} \widetilde{w}' = \mathcal{C}(\widetilde{w} + w) & (\text{Explicit}) \\ w' = \mathcal{D}(\widetilde{w} + w) & (\text{Implicit}) \end{cases} \quad \text{with } v = \widetilde{w} + w, \qquad (1)$$

(order **PRK** $= \min($order **ERK**, order **DIRK**$)$)

Nonlinearly implicit-explicit schemes

- Application of s stages **PRK**

for $i = 1, \dots, s$

$\widetilde{w}^{(i)} = \widetilde{w}^n + \Delta t \sum_{j=1}^{i-1} \widetilde{a}_{ij} \mathcal{C}(\widetilde{w}^{(j)} + w^{(j)})$

solve $w^{(i)} = w^n + \Delta t \sum_{j=1}^{i-1} a_{ij} \mathcal{D}(\widetilde{w}^{(j)} + w^{(j)}) + a_{ii} \mathcal{D}(\widetilde{w}^{(i)} + w^{(i)})$

end

$\widetilde{w}^{n+1} = \widetilde{w}^n + \Delta t \sum_{j=1}^{s} \widetilde{b}_j \mathcal{C}(\widetilde{w}^{(j)} + w^{(j)})$

$w^{n+1} = w^n + \Delta t \sum_{j=1}^{s} b_j \mathcal{D}(\widetilde{w}^{(j)} + w^{(j)})$

- Simplification by setting $v_n = \widetilde{w}_n + w_n$, $v^{(i)} = \widetilde{w}^{(i)} + w^{(i)}$:

for $i = 1, \dots, s$

$$\text{solve } v^{(i)} = v^n + \Delta t \left(\sum_{j=1}^{i-1} \widetilde{a}_{ij} \mathcal{C}(v^{(j)}) + \sum_{j=1}^{i-1} a_{ij} \mathcal{D}(v^{(j)}) + a_{ii} \mathcal{D}(v^{(i)}) \right)$$

end

$$v^{n+1} = v^n + \Delta t \sum_{j=1}^{s} \left(\widetilde{b}_j \mathcal{C}(v^{(j)}) + b_j \mathcal{D}(v^{(j)}) \right)$$

Nonlinearly implicit-explicit schemes

- This algorithm requires solving for $z = v^{(i)}$, $i = 1, \dots, s$, nonlinear systems of M equations ($M = \#\text{PDE} \times \#\text{dof} \gg 0$) as follows:

$$F(z) = z - \mu \mathcal{D}(z) - r = 0, \quad \mu = \Delta t a_{ii} > 0$$

$$r = v^n + \Delta t \left(\sum_{j=1}^{i-1} \widetilde{a}_{ij} \mathcal{C}(v^{(j)}) + \sum_{j=1}^{i-1} a_{ij} \mathcal{D}(v^{(j)}) \right)$$

- Does it have a solution? Is it **unique**?
- For general PDE, + answer only for small enough Δt; in some cases, + answer, for any $\Delta t > 0$ (see **gradient flow**).
- How can we compute it? (direct fixed point method discarded)

Newton's method

- **Damped Newton's method** for solving $F(z) = 0,\ z, F(z) \in \mathbb{R}^M$:

  Input: Initial guess z_0
  for $i = 0, \dots$
  solve for δ_i: $F'(z_i)\delta_i = -F(z_i)$ **(need $\exists F'(z_i)^{-1}$)**
  $z_{i+1} = z_i + \alpha_i \delta_i$, (choice $\alpha_i = 1 \Rightarrow$ Newton's method)
  end

  $\alpha_i \approx \min_{\alpha \in (0,1]} \|F(z_i + \alpha\delta_i)\| \Rightarrow \|F(z_{i+1})\| < \|F(z_i)\|$ ($\approx$ **Armijo's rule**)

- Strictly decreasing **nonlinear residuals**

$$\|F(z_0)\| > \|F(z_1)\| > \dots$$

- **Newton-Kantorovich's theorem $\Rightarrow$ guaranteed fast convergence** (quadratic) $z_i \to z$ if $\alpha_i \to 1$

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Diffusively corrected multi-species kinematic flow models

- We apply in **[Bürger, Mulet, and Villada (2013)]** **Nonlinearly Implicit-Explicit** schemes to:
  - **Polydisperse sedimentation with compression** **[Berres, Bürger, Karlsen, and Tory (2003)]**
  - **Multi-Class LWR traffic model with anticipation and reaction time** **[Wong and Wong (2002); Benzoni-Gavage and Colombo (2003); Bürger, Mulet, and Villada (2013)]**

$$u_t + f^{\mathsf{c}}(u)_x - f^{\mathsf{d}}(u, u_x)_x = 0, u, f^{\mathsf{c}}(u), f^{\mathsf{d}}(u, u_x) \in \mathbb{R}^m.$$

(**1D models**)

- Different species characterized by:
  - Spherical particles with different diameters: $d_1 > \cdots > d_m$
  - Drivers with different maximal velocities: $\beta_1 > \cdots > \beta_m$
- $u_i \equiv$ density of i-th species.

Diffusively corrected multi-species kinematic flow models

- **Kinematic convective fluxes**, for velocities for i-th species $v_i(u)$:

$$f_i^{\mathsf{c}}(u) = u_i v_i(u)$$

where $v_i(u)$ depends globally on all components through few functions (simplifies hyperbolicity analysis through **secular equation [Donat and Mulet (2010)]**)

  - MCLWR (Dick-Greenberg $V_{\mathsf{traf}} \downarrow$)

$$v_i(u) = \beta_i V_{\mathsf{traf}}(\phi), \quad \phi = u_1 + \cdots + u_m.$$

  - Polydisperse sedimentation (MLB model, Richardson-Zaki $V_{\mathsf{sed}} \downarrow$)

$$v_i(u) = \nu(1-\phi)V_{\mathsf{sed}}(\phi)(\delta_i - \sum_j \delta_j u_j), \quad \delta_i = \frac{d_i^2}{d_1^2}.$$

Diffusively corrected multi-species kinematic flow models

- **Strongly degenerate diffusion** for diffusion matrix $A^{\mathsf{d}}(u) \in \mathbb{R}^{m\times m}$:

$$f^{\mathsf{d}}(u, u_x) = A^{\mathsf{d}}(u)u_x, \quad A^{\mathsf{d}}(u) = 0 \text{ for } \phi < \phi_{\mathrm{c}}, \quad \lambda(A^{\mathsf{d}}(u)) \geq 0$$

$(\phi = u_1 + \cdots + u_m \equiv$ **total concentration**$)$

hyperbolic behavior (shocks/rarefactions) on dillute suspensions or light traffic, diffusion only above **threshold** $\phi_{\mathrm{c}} > 0$.

Spatial discretization

- **Convective numerical fluxes**: use Finite-Difference **WENO** schemes **[Shu and Osher (1989)]** applied to **local characteristic** fluxes (more precise although more expensive than **component-wise** application **[Zhang, Wong, and Shu (2006)]**)
- **Diffusive numerical fluxes**: (recall $v_j = v_j(t) \approx u(x_j, t)$)

$$\left(A^{\mathsf{d}}(u)u_x\right)(x_{j+\frac{1}{2}}, t) \approx \overbrace{\frac{1}{2}\left(A^{\mathsf{d}}(v_j) + A^{\mathsf{d}}(v_{j+1})\right)\frac{v_{j+1} - v_j}{\Delta x}}^{\widehat{f}^{\mathsf{d}}(v)_{j+\frac{1}{2}}} \Rightarrow$$

$$\mathcal{D}(v)_j = \frac{\widehat{f}^{\mathsf{d}}(v)_{j+\frac{1}{2}} - \widehat{f}^{\mathsf{d}}(v)_{j-\frac{1}{2}}}{\Delta x} \Rightarrow \mathcal{D}(v) = \Delta x^{-2}\mathcal{B}(v)v,$$

for $\mathcal{B}(v)$ a tridiagonal block matrix, with $m \times m$ blocks which are functions of $A^{\mathsf{d}}(v_j)$.

Continuation strategy for Newton's method

- Diffusion matrix function $A^{\mathrm{d}}(u)$ is not differentiable for $\phi = \sum_{k=1}^{m} u_k = \phi_{\mathrm{c}} \Rightarrow \mathcal{D}(v)$ is not differentiable.
- Standard Newton's method requires differentiable $\mathcal{D}$ $\Rightarrow$ regularize $\mathcal{D}$ by $\varepsilon > 0$:

$$\text{differentiable } \mathcal{D}_\varepsilon \approx \mathcal{D} \quad (\lim_{\varepsilon \to 0} \|\mathcal{D}_\varepsilon - \mathcal{D}\|_\infty = 0)$$

$$\mathcal{D}_\varepsilon(u) = 0, \text{when} \sum_{k=1}^{m} u_k \leq \phi_c$$

(strongly degenerate diffusion also for regularized problems).

- Convergence of (damped) Newton's method **worsens** when $\varepsilon \to 0$
- **Continuation strategy**: obtain u_{ε_0} for large ε_0, decrease ε_0 to ε_1 and use u_{ε_0} as initial guess for Newton method to solve for ε_1 ... until reaching $\varepsilon_{\min} \approx 0$.

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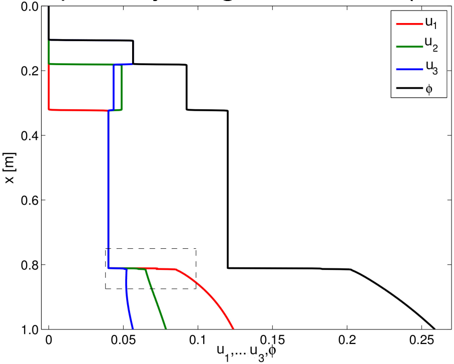
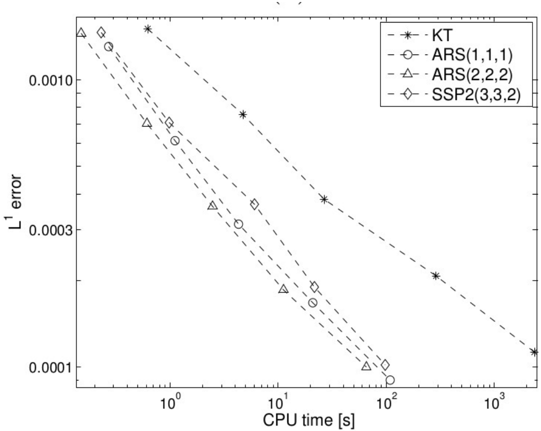
Tridisperse sedimentation with compression

- Use following IMEX-RK schemes:
  - ARS(1,1,1) (1st order), 1 stage **[Ascher, Ruuth, and Spiteri (1997)]**
  - ARS(2,2,2) (2nd order), 2 stages **[Ascher, Ruuth, and Spiteri (1997)]**
  - SSP2(3,3,2) (2nd order), 3 stages **[Pareschi and Russo (2005)]**
- 3 species with diameters $d_1 > d_2 > d_3$ (1 fastest, 3 slowest)
- **Total concentration** $\phi = u_1 + u_2 + u_3$, **threshold** $\phi_c = 0.2$
- Reference soln. computed by Kurganov-Tadmor (KT, explicit) scheme.



Efficiency plot

- Approximate L^1 errors vs CPU for KT (explicit) and IMEX schemes
- All IMEX have approximately the same efficiency, and are more than 10 times faster (for the same accuracy) than KT.



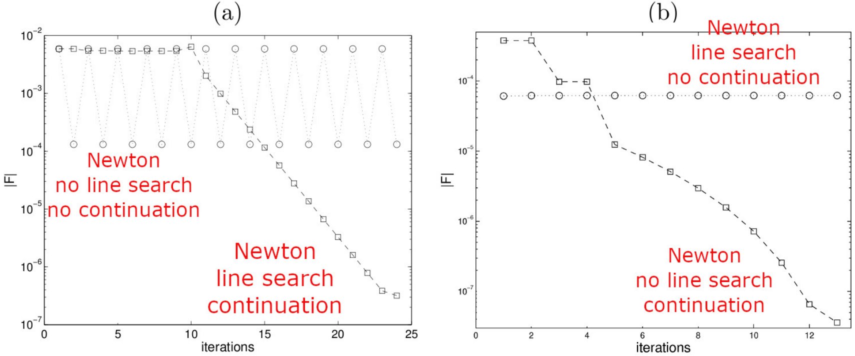
Comparison convergence history for Newton's method

$\|F(z_\nu)\|_2$ vs. iteration count ν for nonlinear solvers (with IMEX-ARS(1,1,1))

$$\text{Newton} \times \left\{ \begin{array}{c} \text{line search} \\ \text{no line search} \end{array} \right\} \times \left\{ \begin{array}{c} \text{continuation} \\ \text{no continuation} \end{array} \right\}$$

Line search: damping with selected α_ν for sufficient decrease or set $\alpha_\nu = 1$

Continuation: gradual decrease $\varepsilon \to \varepsilon_{\min} \approx 0$ or fixed $\varepsilon_{\min}$.



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Linearly implicit-explicit schemes

- Although NIMEX schemes revealed to be quite robust in our tests, the cost per iteration (and implementation) is not trivial.
- **[Boscarino, Bürger, Mulet, Russo, and Villada (2015)]** Apply PRK scheme to system obtained by **doubling variables** (recall $\mathcal{D}(v) = \Delta x^{-2}\mathcal{B}(v)v$ and that stiffness does not come from $\mathcal{B}(v)$, but from Δx^{-2})

$$v' = \mathcal{C}(v) + \Delta x^{-2}\mathcal{B}(v)v, v(0) = v^0$$

$$\iff \begin{cases} \widetilde{v}' = \mathcal{C}(\widetilde{v}) + \Delta x^{-2}\mathcal{B}(\widetilde{v})v, \widetilde{v}(0) = v^0 \\ v' = \mathcal{C}(\widetilde{v}) + \Delta x^{-2}\mathcal{B}(\widetilde{v})v, v(0) = v^0 \end{cases}$$

- Specifically, apply an explicit RK scheme (with Butcher array $\widetilde{A}, b$) to the $\widetilde{v}$ variable and a DIRK scheme (with Butcher array A, b) to the v variable (same b vectors), both of s stages.

Linearly implicit-explicit schemes

- Using the notation $\Phi(\widetilde{v}, v) = \mathcal{C}(\widetilde{v}) + \Delta x^{-2}\mathcal{B}(\widetilde{v})v$:

  for $i = 1, \dots, s$

  $\widetilde{v}^{(i)} = v^n + \Delta t \sum_{j=1}^{i-1} \widetilde{a}_{ij}\Phi(\widetilde{v}^{(j)}, v^{(j)})$ **(explicit)**

  $v^{(i)} = v^n + \Delta t \sum_{j=1}^{i-1} a_{ij}\Phi(\widetilde{v}^{(j)}, v^{(j)}) + \Delta t a_{ii}\Phi(\widetilde{v}^{(i)}, v^{(i)})$ **(implicit)**

  end

  $v^{n+1} = v^n + \Delta t \sum_{j=1}^{s} b_j \Phi(\widetilde{v}^{(j)}, v^{(j)})$

- Only need to solve, for each i, the **linear equation** in $v^{(i)}$

$$(I - \frac{\Delta t a_{ii}}{\Delta x^2}\mathcal{B}(\widetilde{v}^{(i)}))v^{(i)} = v^n + \Delta t \left(\sum_{j=1}^{i-1} a_{ij}\Phi(\widetilde{v}^{(j)}, v^{(j)}) + \Delta t a_{ii}\mathcal{C}(\widetilde{v}^{(i)}) \right)$$

- Memory can be saved by storing, using and solving directly (same matrix, different right hand) for the variables $K_j = \Phi(\widetilde{v}^{(j)}, v^{(j)})$ (**no penalty paid for doubling variables, half memory requirements**).

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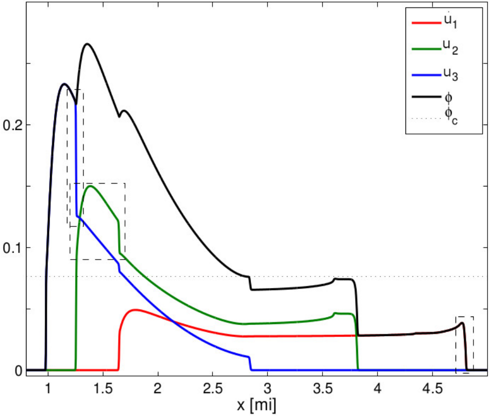
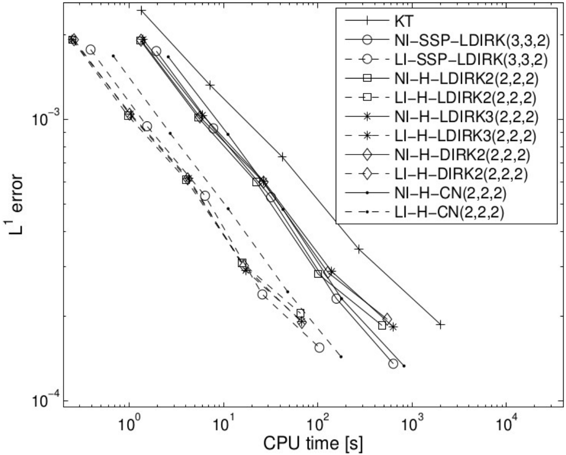
3-Class Lighthill-Whitham-Richards traffic model

- Comparison of NIMEX vs LIMEX for **sedimentation**: **NIMEX is more accurate and LIMEX cheaper per iteration and have ≈ same efficiency.**
- Simulation $T = 3\text{min}$, 5 miles circular road (periodic B.C.)
- $u_1 \equiv$ fastest drivers, $u_3 \equiv$ slowest drivers (normalized units, $1 =$ bumper to bumper)
- Diffusion threshold $\phi_c = 0.075$



3-Class Lighthill-Whitham-Richards traffic model

LIMEX schemes in test: H-CN(2,2,2) H-DIRK2(2,2,2) H-LDIRK$\{2,3\}$(2,2,2) SSP-LDIRK(3,3,2)



Efficiency plot (approximate L^1 errors vs CPU) $\Rightarrow$ LIMEX almost $10\times$ faster than corresponding NIMEX in this case.

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Gradient flow equations

- **Goal:** efficient numerical solution of PDE with **gradient flow structure** **[Carrillo, Chertock, and Huang (2015); Burger, Fetecau, and Huang (2014)]**

$$
\begin{aligned}
&u_t + \nabla \cdot \left(f^{\mathsf{c}}[u] - f^{\mathsf{d}}[u] \right) = 0, \\
&f^{\mathsf{c}}[u] = u \nabla (W * u), \quad \textbf{convective flux} \text{ (nonlocal, convolution)} \\
&f^{\mathsf{d}}[u] = u \nabla (H'(u)), \quad \textbf{diffusive flux}
\end{aligned}
$$

  - $0 \leq u(x,t) \equiv$ **population density**, space$\equiv x \in \mathbb{R}^m$, time $\equiv t$
  - $W(x) \equiv$ (symmetric) **interaction potential**,
  - $H(u) \equiv$ (convex) density of **internal energy**.
- Models **collective behavior**, **interacting gases**, **porous media flow**, ...

Gradient flow equations

- Assume smooth enough interaction potential W, so that

$$f^{\mathsf{c}} = u\nabla(W * u) = u((\nabla W) * u)$$

depends nonlocally on u.

- **[Bürger, Inzunza, Mulet, and Villada (2019)]** Rewrite diffusive flux as:

$$f^{\mathsf{d}}[u] = u\nabla(H'(u)) = uH''(u)\nabla u \Rightarrow K(u) = \int_0^u sH''(s)ds \Rightarrow$$
$$K'(u) = uH''(u) \geq 0 \Rightarrow \nabla K(u) = K'(u)\nabla u = f^{\mathsf{d}}[u]$$

so that $\nabla \cdot f^{\mathsf{d}}[u] = \nabla \cdot \nabla K(u) = \Delta K(u)$

- **Degenerate diffusion:** $u(x) = 0 \Rightarrow K'(u(x)) = K'(0) = 0$
- **Example:** $H(u) \propto u^\eta \Rightarrow K(u) \propto u^\eta$ $\begin{cases} \text{fast diffusion} & \eta < 1 \\ \text{slow diffusion} & \eta > 1 \end{cases}$

Numerical fluxes ([Carrillo, Chertock, and Huang (2015)])

- Consider $f^{\mathsf{c}}[u] = u(W * u - H'(u))_x$, $f^{\mathsf{d}} = 0$ ($\Rightarrow \mathcal{D} = 0$) and compute

$$\widehat{f}^{\mathsf{c}}(v)_{j+1/2} = \widetilde{v}_{j+1/2}\widetilde{w}_{j+1/2},\ \widetilde{w}_{j+1/2} = \frac{\widetilde{G}_{j+1} - \widetilde{G}_j}{\Delta x}, \widetilde{G}_j = (W *_h v)_j - H'(v_j)$$

(discrete convolutions $*_h$ computed by **FFT, key to performance**)

$$\widetilde{v}_{j+1/2} = \begin{cases} \mathsf{MUSCL}(v_{j-1}, v_j, v_{j+1}) & \widetilde{w}_{j+1/2} > 0 \\ \mathsf{MUSCL}(v_j, v_{j+1}, v_{j+2}) & \widetilde{w}_{j+1/2} < 0 \end{cases}$$

MUSCL $\equiv$ upwind, 2nd order, $+$preserv reconstruction

Numerical fluxes ([Bürger, Inzunza, Mulet, and Villada (2019)])

- Based on **[Donat, Guerrero, and Mulet (2018)]**, use **decoupled discretizations**: $f^{\mathsf{c}}[u] = u(W * u)_x \Rightarrow$

$$\widehat{f^{\mathsf{c}}}(v)_{j+1/2} = v_{j+1/2} w_{j+1/2}, \quad w_{j+1/2} = \frac{G_{j+1} - G_j}{\Delta x}, G_j = (W *_h v)_j$$

$$v_{j+1/2} = \begin{cases} \mathsf{MUSCL}(v_{j-1}, v_j, v_{j+1}) & w_{j+1/2} > 0 \\ \mathsf{MUSCL}(v_j, v_{j+1}, v_{j+2}) & w_{j+1/2} < 0. \end{cases}$$

- $\mathcal{D}(z) = \Delta_h \boldsymbol{K}(z)$, $\boldsymbol{K}(z)_j = K(z_j)$, with standard Laplacian Δ_h, Dirichlet b.c. (**compactly supported solution**).

Explicit schemes

Theorem ([Carrillo, Chertock, and Huang (2015)])

Under the CFL condition $\dfrac{\Delta t}{\Delta x} \max_j |\widetilde{w}_{j+1/2}| \leq \dfrac{1}{2}$, *the Explicit Euler's Method is* $+$*preserving.*

Theorem ([Bürger, Inzunza, Mulet, and Villada (2019)])

Under the CFL condition $\Delta t \left(\dfrac{\max_j |w_{j+1/2}|}{\Delta x} + \dfrac{\max\limits_{0 \leq u \leq \|v\|_\infty} K'(u)}{\Delta x^2} \right) \leq \dfrac{1}{2}$,

EEM is $+$*preserving.*

- CFL $\Rightarrow$ $+$preserving explicit schemes obtained by **SSP-RK3** (convex combination of 3 EE steps)
- $\max_j |w_{j+\frac{1}{2}}| = \mathcal{O}(1)$ (if W smooth enough)
- $\max_j |\widetilde{w}_{j+\frac{1}{2}}| = \mathcal{O}(\Delta x^{-1}) \Rightarrow \Delta t = \mathcal{O}(\Delta x^2)$ for both schemes.

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Nonlinearly Implicit-Explicit schemes

- Applying LIMEX would ruin "nice" structure of diffusion $\Delta K(u)$.
- Recall that the NIMEX-RK algorithm requires solving for $z = v^{(i)}$, $i = 1, \dots, s$, nonlinear systems of M equations ($M = \#\text{PDE} \times \#\text{dof} \gg 0$) as follows:

$$F(z) = z - \mu \mathcal{D}(z) - r = 0, \quad \mu = \Delta t a_{ii} > 0,$$
$$r = \text{(known) vector built from previous RK stages}$$

- Use special structure of $\mathcal{D}(z) = \Delta_h \boldsymbol{K}(z)$, $\boldsymbol{K}(z)_j = K(z_j)$ to prove:

Theorem ([Bürger, Inzunza, Mulet, and Villada (2019)])

$\mu > 0$, $r \in \mathbb{R}^M$, $r_j \geq 0$, $j = 1, \dots, M \Rightarrow$ *the equation*

$$z - \mu \mathcal{D}(z) - r = 0$$

has a unique solution $z \in \mathbb{R}^M$ *satisfying* $z_j \geq 0$, $j = 1, \dots, M$.

Nonlinearly Implicit-Explicit schemes

- Previous result (based on Brouwer's fixed point Theorem) applies to get:

Theorem ([Bürger, Inzunza, Mulet, and Villada (2019)])

Under the CFL condition $\boxed{\dfrac{\Delta t}{\Delta x} \max_j |w_{j+1/2}| \leq 1/2}$ *the Euler IMEX method*

$$v^{n+1} = v^n + \Delta t\big(\mathcal{C}(v^n) + \mathcal{D}(v^{n+1})\big)$$

is a positivity preserving scheme.

Sketch of proof

- $v^n \geq 0$ + CFL $\Rightarrow v^n + \Delta t\mathcal{C}(v^n) \geq 0$ (by theorem on explicit scheme)
- Previous theorem applied to $v^{n+1} - \underbrace{\Delta t}_{\mu} \mathcal{D}(v^{n+1}) - \underbrace{(v^n + \Delta t\mathcal{C}(v^n))}_{r} = 0$ yields $\exists!$ solution $v^{n+1} \geq 0$.

Nonlinearly Implicit-Explicit schemes

- Tried Shu-Osher SSP strategy **[Shu and Osher (1988)]** to get second order accuracy, e.g.:

$$\begin{aligned}
v^{(1)} &= v^n + \gamma_1 \Delta t \big(\mathcal{C}(v^n) + \mathcal{D}(v^{(1)})\big) \\
v^{(2)} &= v^{(1)} + \gamma_2 \Delta t \big(\mathcal{C}(v^{(1)}) + \mathcal{D}(v^{(2)})\big) \\
v^{n+1} &= (1-\alpha) v^{(1)} + \alpha v^{(2)}, \\
0 &< \alpha \leq 1, \gamma_1, \gamma_2 > 0
\end{aligned}$$

  but $\nexists$ such $\alpha, \gamma_1, \gamma_2$. $\Rightarrow$ no direct application to higher-order IMEX-RK schemes ($\nexists$ RK implicit schemes in SSP form of order > 1 **[Gottlieb, Shu, and Tadmor (2001)]**).
- No problems in our numerical experiments with 2^{nd} order non-SSP versions, but would like to explore other strategies for $+$ preserving schemes of order > 1.

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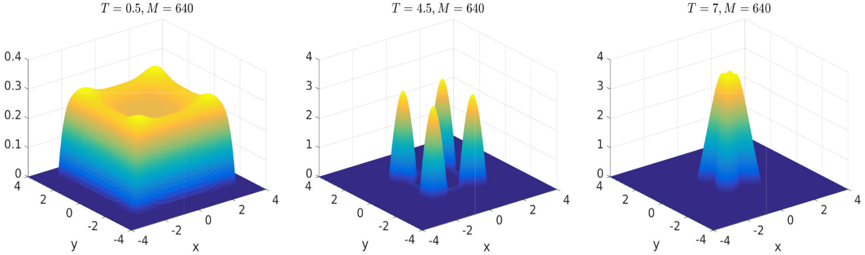
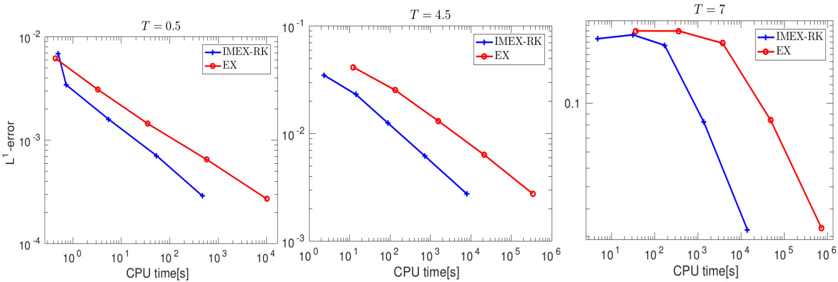
2D experiments

- Test from **[Carrillo, Chertock, and Huang (2015)]** (smooth interaction potential, slow diffusion)

$$u_0 = 0.25\chi_{[-3,3]\times[-3,3]},$$
$$W(x_1,x_2) = \frac{1}{\pi}\exp(-x_1^2 - x_2^2),$$
$$H(u) = \frac{\nu}{\eta}u^\eta, \nu = 0.1, \eta = 2.1$$



Efficiency plot (approximate L^1 errors vs. CPU)

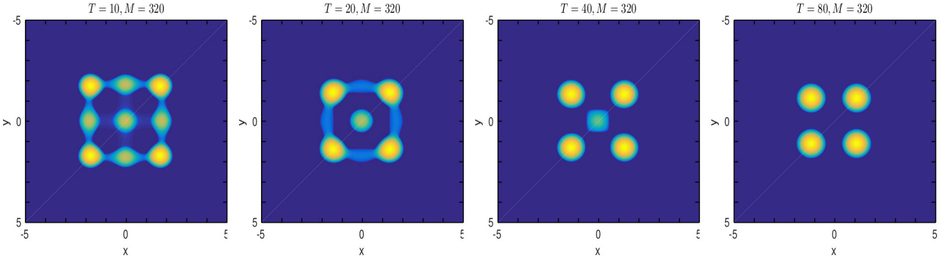


- CPU gain of IMEX with respect to explicit scheme **[Carrillo, Chertock, and Huang (2015)]** ranges from 10 to 100 in this case (gap, of course, increases with resolution)

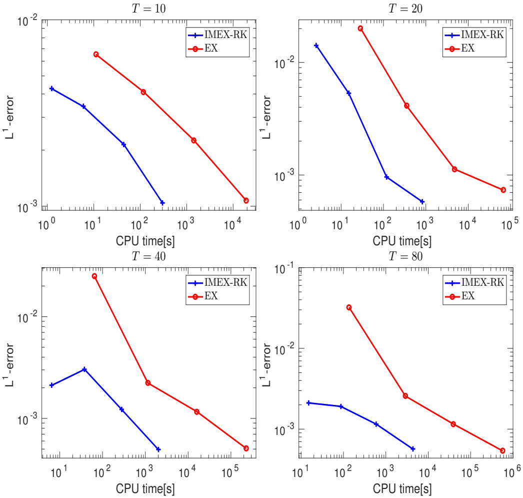
2D experiments

- Test from **[Carrillo, Chertock, and Huang (2015)]** (non-smooth interaction potential, slow diffusion)

$$
\begin{aligned}
u_0 &= 0.05\chi_{[-3,3]\times[-3,3]}\\
W(\boldsymbol{x}) &= -(1-|\boldsymbol{x}|)_+,\\
H(u) &= \frac{\nu}{\eta}u^\eta, \nu = 1.48, \eta = 3.
\end{aligned}
$$



Efficiency plot (approximate L^1 errors vs. CPU)



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Conclusions

- Can get efficient RK numerical methods by treating implicitly some (but not all) terms in the spatial discretization in MOL applied to PDE with convection and degenerate diffusion.
- Can get order > 1 both for Nonlinearly-IMEX and Linearly-IMEX.
- LIMEX is much easier to implement and the cost per step is smaller than NIMEX, but these may be preferable for some favorable structures.
- When using Newton's method continuation (in some limited cases) and line-search strategies might be worthy for ensuring convergence.
- Have used these methods for some diffusively corrected kinematic models and gradient flow models.

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Interacting species with cross-diffusion

- Model in **[Carrillo, Filbet, and Schmidtchen (2018); Carrillo, Huang, and Schmidtchen (2018)]** for interacting species with nonlocal behavior:

$$\begin{cases} \dfrac{\partial u_1}{\partial t} = \dfrac{\partial}{\partial x}\left(u_1 \dfrac{\partial}{\partial x}\left(W_{11} * u_1 + W_{12} * u_2 + \nu(u_1 + u_2)\right) + \dfrac{\epsilon}{2}\dfrac{\partial u_1^2}{\partial x}\right), \\ \dfrac{\partial u_2}{\partial t} = \dfrac{\partial}{\partial x}\left(u_2 \dfrac{\partial}{\partial x}\left(W_{22} * u_2 + W_{21} * u_1 + \nu(u_1 + u_2)\right) + \dfrac{\epsilon}{2}\dfrac{\partial u_2^2}{\partial x}\right), \end{cases}$$

  W_{11}, W_{22} are **self-interaction potentials** and W_{12}, W_{21} are **cross-interaction potentials**, $\nu > 0$ is the coefficient of cross-diffusivity and ε the coefficient of self-diffusivity.

- Treat implicitly diffusion terms.

Navier-Stokes-Cahn-Hilliard equations

- **[Lowengrub and Truskinovsky (1998); Abels and Feireisl (2008)]** Models evolution of compressible mixture of **binary fluids** (e.g. foams, solidification processes, fluid–gas interface, ...) under gravity.
- $c \equiv$ concentration of 1st species, $\rho \equiv$ density of mixture, $v \equiv$ velocity, $G \equiv$ gravitational acceleration, $p(\rho, c) \equiv$ pressure, $\varepsilon, \nu_{\mathsf{NS}}, \nu_{\mathsf{CH}} > 0$.

$$\rho_t + \nabla \cdot (\rho v) = 0$$

$$(\rho v)_t + \nabla \cdot (\rho v \otimes v + p(\rho, c) I) = \rho G + \nu_{\mathsf{NS}} \left(\Delta v + \frac{1}{3} \nabla \nabla \cdot v \right)$$

(2)

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$$
\begin{aligned}
\rho_t + \nabla \cdot (\rho v) &= 0 \\
(\rho v)_t + \nabla \cdot (\rho v \otimes v + p(\rho, c) I) &= \rho G + \nu_{\mathsf{NS}} \left(\Delta v + \frac{1}{3} \nabla \nabla \cdot v \right) \\
&\quad - \varepsilon \nabla \cdot (\rho \nabla c \otimes \nabla c) \\
(\rho c)_t + \nabla \cdot (\rho c v) &= \nu_{\mathsf{CH}} \Delta \left(\mu_0(\rho, c) - \frac{\varepsilon}{\rho} \nabla \cdot (\rho \nabla c) \right) \qquad (2)
\end{aligned}
$$

- Treat implicitly these terms, specially that in (2) (solving this Cahn-Hilliard equation explicitly would require $\Delta t \propto \Delta x^4$!)

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