Implicit Temporal Methods for Entropy Stable Spectral Collocation

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- Old Dominion: Nail Yamaleev

The View from 35,007’

The “Whole Package” matters!

Given spatial discretization, important elements of an integrator are:

- The main integration scheme : $\mathbf{U}^n \rightarrow \mathbf{U}^{n+1}$
  - Implicit: Stepwise & internal A- & L-stability, (E)SDIRK
  - Explicit: Runge-Kutta
- Peripheral temporal components
  - Stage-Value-Predictors : $\tilde{\mathbf{U}}^{(j)}$ Starts Nonlinear iteration!!!!
  - Embedded error estimate : $\hat{\mathbf{U}}^{n+1}$
  - Controller
    - Timestep adjustment (track error $||\epsilon|| = ||\mathbf{U}^{n+1} - \hat{\mathbf{U}}^{n+1}||$)
    - Iteration termination (don’t oversolve) Söderland
    - Reevaluate preconditioner Jacobian (only when needed)
- Solver: Linear/Nonlinear
  - Weakest link for high-order spatial/temporal schemes
    - Parallel partitioning strategies
    - Local / Global preconditioner(s)
    - H-O (DG) operators are horribly conditioned!

Do the “Unthinkable”: Add more Runge-Kutta stages!

- With more stages in main Runge-Kutta Scheme : $\mathbf{U}^{n+1}$ can we
  - Lessen burden on implicit linear/nonlinear solver mechanics?
    - Build schemes with better internal properties (accuracy/conditioning/error estimates)?
    - Build better Stage-Value predictors?
    - More controllability
- Are they more efficient than state-of-art 3rd-order RK integrators?
  - IMEX3(2)4L[2]SA (KC: ANM 2003)
    - Vogl, Steyer, Reynolds, Ullrich, Woodward, JAMES (J...Earth Sci), 10.1029/2019MS001700

Motivating Problems of Interest

Technical Challenge: Develop robust tools for predicting aerodynamic stall, buffet, flutter and propulsion system performance

- RANS: existing models are reliable for portions of design space
- RANS: NOT RELIABLE for unsteadiness around perimeter of envelope! (e.g., Low-speed/High-lift, stall, buffet, flutter, propulsion systems)
- Currently, higher fidelity unsteady simulation tools are necessary (e.g., LES)

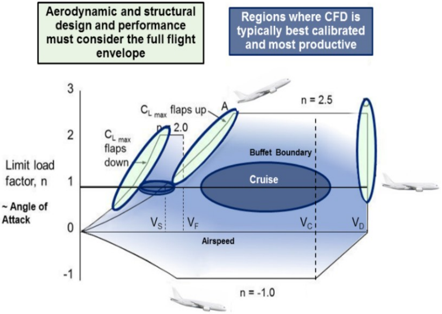


Figure: Load Factor/Airspeed Flight Envelope.

High-Order (H-O) spatial operators and numerical methods

- Entropy Conservative/Stable Spectral Collocation for Navier-Stokes
  - Enables stronger statements on integral stability of numerical solution (albeit incomplete)

But which temporal scheme?

- Stiffness $\rightarrow$ Implicit methods (A-stability, L-stability)
  - High-aspect ratio boundary elements: e.g., 1000:1:1
  - Physical scale separation: e.g., vortex generators in BL
  - Defective grid generation: e.g., sliver cells/elements
  - Point singularities: sharp trailing edge refinement
  - Source terms: Chemistry or turbulence models

An Ocean of Integrators: Automated Integration

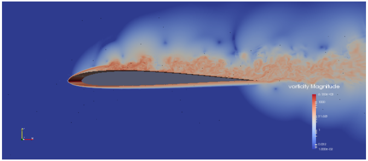
- Multipurpose integrator CFD: Linear Multistep, MultiStage, GLM
  - External Aero: nonstiff / stiff / separably stiff (IMEX, multirate)
- Unique Algorithmic Constraints
  - Adaptive Mesh Refinement → Self-starting → Runge-Kutta
    - Refinement transmission conditions: difficult for HO methods
    - Multistep transmission condition ???????? Not today!
  - Implicit RK: Stepwise & internal A- & L-stability → Robustness
  - Amenable to implicit/explicit partitioning → Efficiency
  - And the verdict is? IMEX (E)SDIRK Runge-Kutta schemes
- Lessons learned with (E)SDIRK Schemes
  - H-O accuracy → multiple stages → mandates huge timesteps
  - Factor 20 larger timestep (relative to BDF2)
  - Whack-a-mole: Increased burden on linear/nonlinear solver
- Potentially a problem with HO spatial discretizations?

A Complimentary Strategy for H-O solvers

- The main integration scheme : $\mathbf{U}^n \rightarrow \mathbf{U}^{n+1}$
  - Stepwise & internal A- & L-stability, (E)SDIRK
  - (E)SDIRK characterized by γ on diagonal of Butcher tableau
    - γ : $\iff$ $(\mathbf{I} + \gamma \Delta t \frac{\partial R}{\partial U})\, \delta U = R(U)$
    - Increase stages by one
    - Minimize γ, $\rightarrow$ better matrix conditioning
    - Optimize error coefficient to allow larger timesteps
- Peripheral temporal components
  - Stage-Value-Predictors: $\tilde{\mathbf{U}}^{(j)}$, used to start nonlinear iteration
    - Study SVP accuracy vs. internal stability tradeoff
    - Design SVP to be A-stable when possible
  - Embedded Error estimate : $\hat{\mathbf{U}}^{n+1}$
  - Controller
    - Timestep adjustment (track error $||\epsilon|| = ||\mathbf{U}^{n+1} - \hat{\mathbf{U}}^{n+1}||$)
    - Iteration termination (don't oversolve) Söderland
    - Reevaluate preconditioner Jacobian (only when needed)
- Can additional stage result in better efficiency?

Baseline NASA LaRC Mechanics

Applications $\rightarrow$ "Productionized" Algorithm



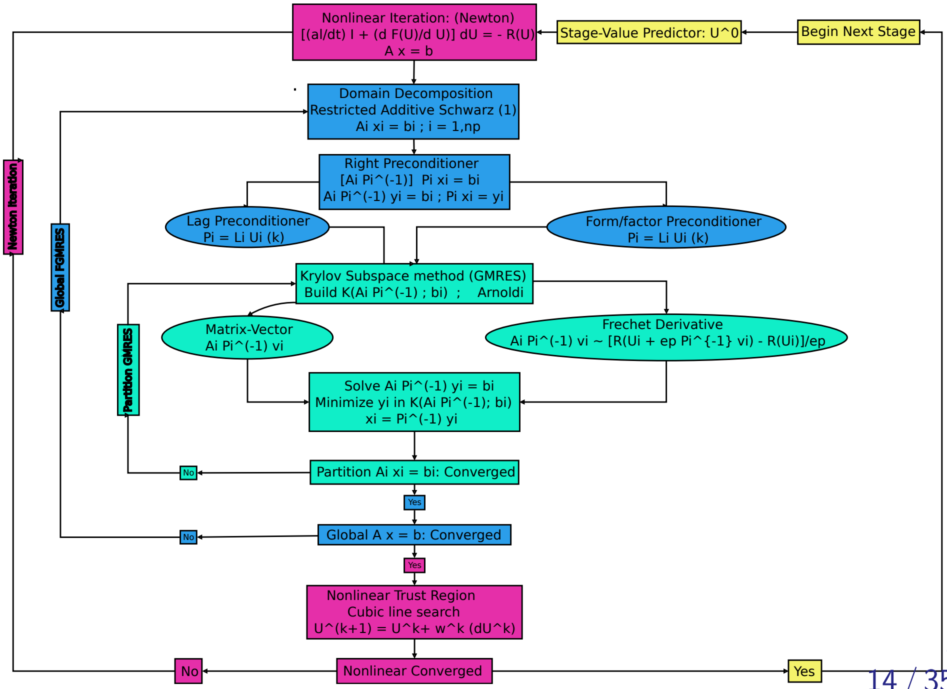
- Spatial Operator: Entropy dissipative Spectral Collocation
  - Curvilinear Hexahedral Elements: Focus on $P1$ - $P7$
  - Conforming / Nonconforming interfaces
  - H- & P-refinement capability
  - Several Dissipation Kernels
- Temporal Operator: Implicit-Explicit Runge-Kutta
  - 3^{rd}- & 4^{th}-order IMEX Runge-Kutta : Stage-order 2
  - Explicit Singly Diagonally Implicit RK (ESDIRK) Implicit
  - Stepwise and Internal A- & L-stability
  - Error estimator / Stage-Value-Predictors (SVP)
- Solver Mechanics: PETSC infrastructure

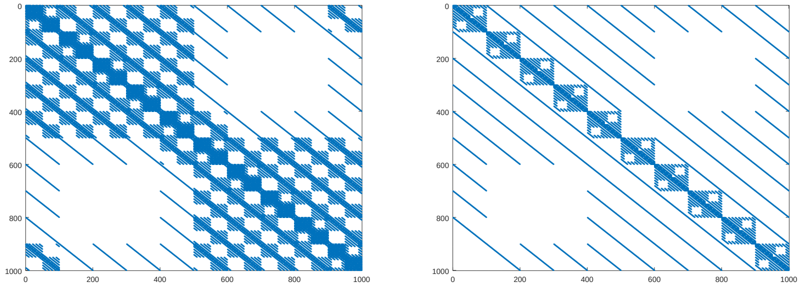
PETSC Solver Mechanics: Details

PETSc Solvers: Another talk for another day!

- Conventional Architecture: 1.5GB/process
- Solver Mechanics: PETSC infrastructure
  - Preconditioned “Reduced-Jacobian”, Newton-Krylov
  - Classical Dom-Decomp: Additive-Schwarz (1 layer overlap)
  - Classical parallel “Inner-Outer” Krylov Iteration (Saad ’93, Van Der Vorst, Vuik ’94)
    - Inner: Partitions each run preconditioned GMRES
    - Approximate Preconditioning matrix: Thin-layer NS
    - Preconditioner: ILU(k), k=0,1,2
    - Stored ILU factors: 10-20 Newton Iterations
    - Arnoldi subspace $AV^n = \bar{V}^{n+1}\bar{H}$ using Frechet derivatives
    - Outer: Flexible GMRES
  - Newton Update
    - Trust-Region / line search
    - Stage-value-predictor used at beginning of each RK stage

PETSC: Nonlinear/Linear "Inner-Outer" Solver



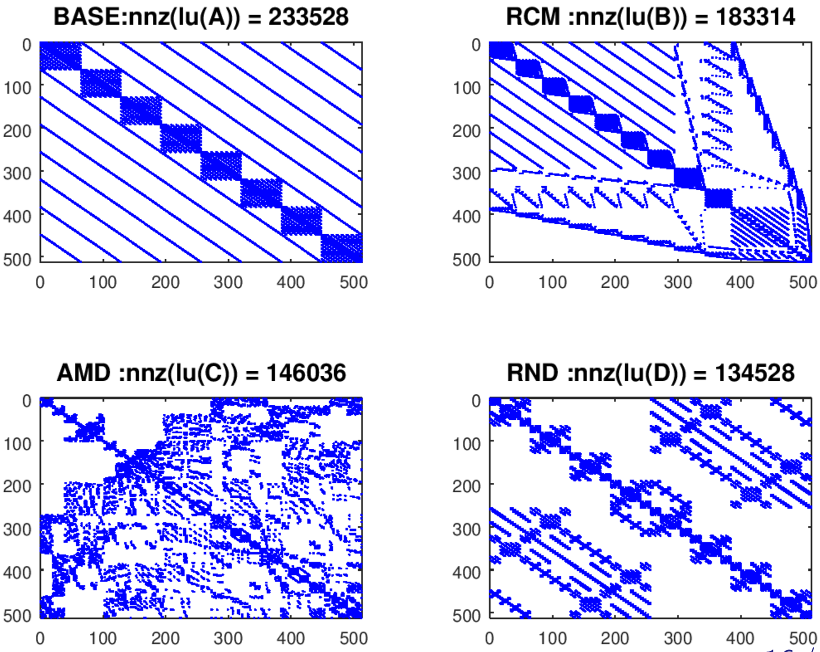


Spy: Full NS VS. Thin-Layer NS. 2x2x2 Periodic. P4 Elements

PolyOrder	*NNZ(Full)*	*MB/Elem*	*NNZ(Thin)*	*MB/Elem*
1	164	0.0082	68	0.0034
2	954	0.0477	378	0.0189
3	3520	0.1760	1168	0.0584
4	10010	0.5005	2750	0.1375
5	24036	1.2018	5508	0.2754
6	50701	2.5350	10045	0.5022
7	97364	4.8682	16448	0.8224

Storage (Mega-Bytes) per element: Full and Thin layer preconditioner

Thin-Layer NS Reordering Strategies



Temporal Mechanics

The Case for "Solver Optimized" Schemes: Free Lunch?

- Design "Solver Optimized" ESDIRK IMEX Runge-Kutta schemes
  - Add additional stage(s): Optimized properties offset cost penalty
- Main design considerations: 1) Accuracy and 2) Condition of solver
  - Accuracy: For $\Uparrow \Delta t$, need $\Downarrow$ T.E.

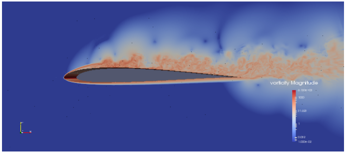
Name	4(3)6L[2]SA	4(3)7L[2]SA
s	6	7
T.E. $A^{(5)}$	0.01224	0.000260

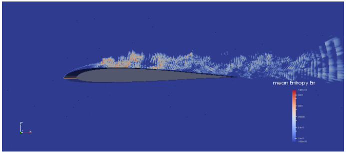
  - Conditioning: Diag Coeffs γ : $\iff$ $\left(\mathbf{I} + \gamma \Delta t \frac{\partial R}{\partial U}\right) \delta U = R(U)$
    - BDF1: $\gamma = 1$,
    - BDF2: $\gamma = \frac{3}{2}$,
    - ESDIRK3(2)4L[2]SA: $\gamma = 0.43$,
    - ESDIRK4(3)6L[2]SA: $\gamma = \frac{1}{4}$
    - Solver Optimized: ESDIRK4(3)7L[2]SA: $\gamma = \frac{1}{8}$
      NASATM:219173, ANM(136):2019, ANM(146):2019
- Free Lunch! "A wash" for $(\Delta t)_{4(3)6} \approx (2\Delta t)_{4(3)7}$

Peripheral Considerations: Stage-Value-Predictors/Error Estimation/Controllers

- SVP: Long History in RK literature (NASATM:219173)
  - Hairer & Wanner, Laburta, Higueras & Roldán, Roldán, Gonzáles-Pinto, Calvo, Olsson & Söderland, $\cdots$
  - Design: delicate balance of accuracy and stability constraints
    - Number of stages determine accuracy of stages
    - Internal L-stability of $\mathbf{U}^n \rightarrow \mathbf{U}^{n+1}$
- Error Estimators $||\epsilon|| = ||\mathbf{U}^{n+1} - \hat{\mathbf{U}}^{n+1}||$
- Controller (NASATM:219173)
  - Söderland's PPID
    $$(\Delta t)^{[n+1]} = \kappa \, (\Delta t)^{[n]} \left\{ \frac{tol}{||\epsilon^{[n+1]}||} \right\}^{\alpha} \left\{ \frac{||\epsilon^{[n+0]}||}{tol} \right\}^{\beta} \left\{ \frac{tol}{||\epsilon^{[n-1]}||} \right\}^{\gamma} \left\{ \frac{(\Delta t)^{[n]}}{(\Delta t)^{[n-1]}} \right\}$$
    $\alpha = +\frac{0.30}{\hat{p}}$, $\beta = -\frac{0.05}{\hat{p}}$, $\gamma = -\frac{0.25}{\hat{p}}$, tol $=$ user input
  - tolerance (tol) set to $10^{-3}, 10^{-4}, 10^{-5}$
  - Used for all tests with a-priori NO TUNING

The Test Case and Preliminary Testing





- High-order workshop III, very popular test case
- $\mathrm{Re}_{ch} = 60K, Pr = 0.72, M = 0.20, AOA = 8.0^\circ$
- Hex meshes (DOF): 14502 (3M), 55008 (11M), 116016 (25M)
  - Eyeball initial mesh → Spatial error estimator → Adjust mesh
- Stiffness: Inadequate GMSH skills

PolyOrd	$(\Delta t)_{max}$
$P1$	$9.0e-6$
$P2$	$1.5e-6$
$P3$	$4.8e-7$
$P4$	$2.0e-7$
$P5$	$9.7e-8$
$P6$	$5.2e-8$

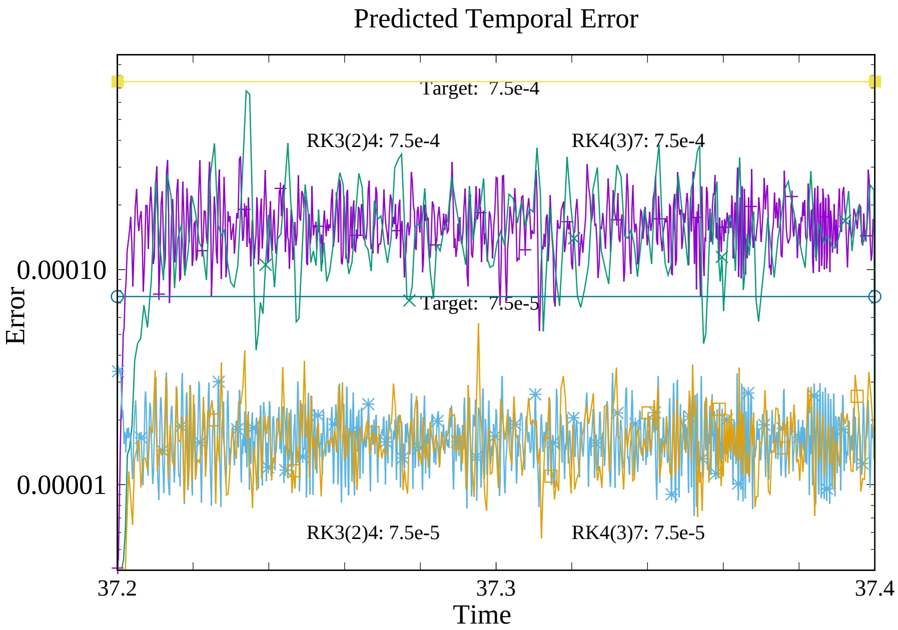
Maximum explicit timestep

Preliminary Test I: Efficacy of Controller

Can controller maintain the specified error tolerance for all schemes?
Critical capability for impartial comparison between schemes.

- SD7003: 116016 Hexahedral elements run at P3
- Tol = 7.5e-5 , 7.5e-4
- Test at Engineering error tolerances: e.g., tol = 7.5e-4 / timestep
  HUGE ERROR (3-4 significant digits in lift and/or Drag)
- Test ONLY IMPLICIT operator from each IMEX pair
- Schemes:
  - IMEX3(2)4L[2]SA (KC: ANM 2003)
  - IMEX4RK(3)7L[2]SA (KC: ANM 2019a)
  - ESDIRK4(3)7L[2]SA (KC: ANM 2019b)

Efficacy of Controller: Maintaining Target Error

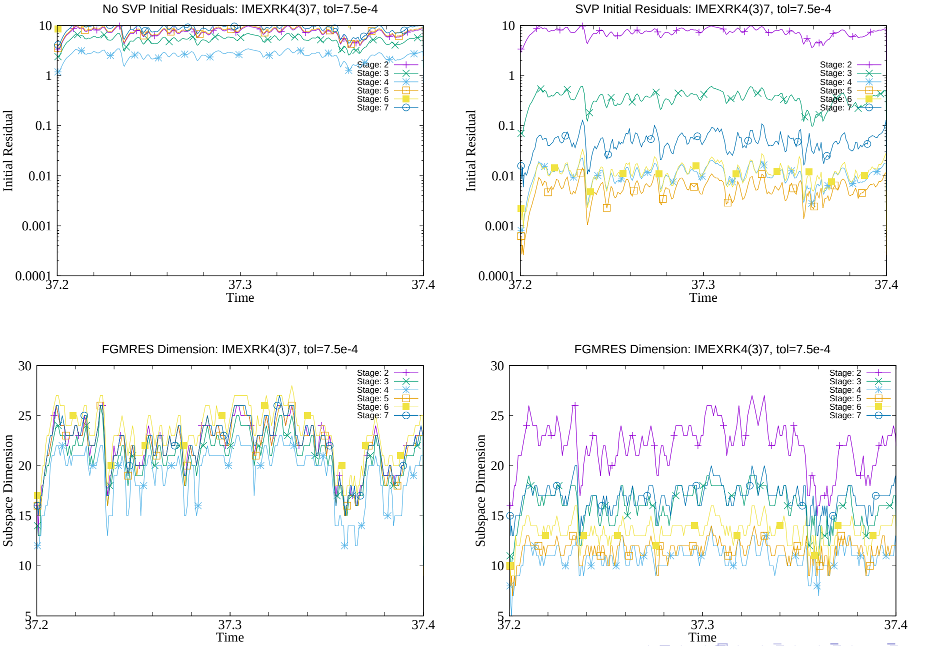


Preliminary Test II: Efficacy of Stage-Value-Predictors

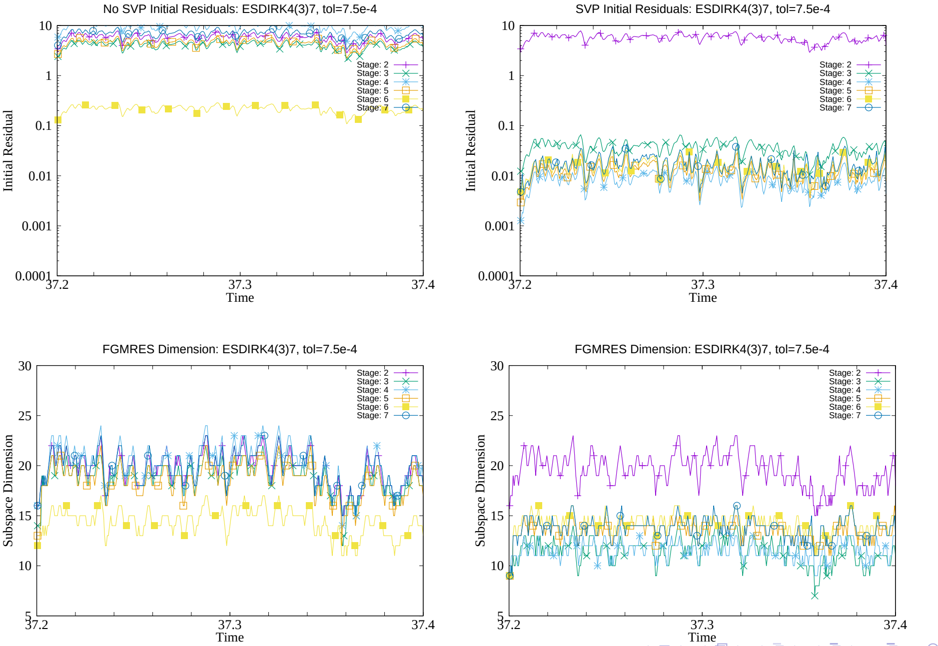
Do SVP reduce time-to-solution of all schemes?

- SD7003: 116016 Hexahedral elements run at P3
- tol = 7.5e-4
- Engineering error tolerance: tol = 7.5e-4 / timestep
  HUGE ERROR (3 significant digits in lift and/or Drag)
- Testing ONLY IMPLICIT portion of each IMEX pair
- Schemes used in Testing
  - IMEXRK4(3)7L[2]SA (Solver Optimized)
  - ESDIRK4(3)7L[2]SA (Solver Optimized)

Convergence WITHOUT and WITH SVP: IMEXRK4(3)7



Convergence WITHOUT and WITH SVP: ESDIRK4(3)7



Efficacy of Controller and SVP: The Verdict is?

- Controller drives all schemes as advertised!
- Always run with the Stage-Value-Predictor!

Scheme	*WITHOUT SVP*		*WITH SVP*		*COST*
	CPUTime	*Steps*	*CPUTime*	*Steps*	*Ratio*
*IMEXRK*4(3)7	52990	245	34577	245	0.65
*ESDIRK*4(3)7	48997	311	33799	314	0.68

- Results consistent with those seen in past work
- Rapid convergence USUALLY correlates with initial residual reduction
- Multiple step SVP for variable time-stepping: i.e., Stage 2,3
- More work to be done to optimize A-stability / accuracy of SVP

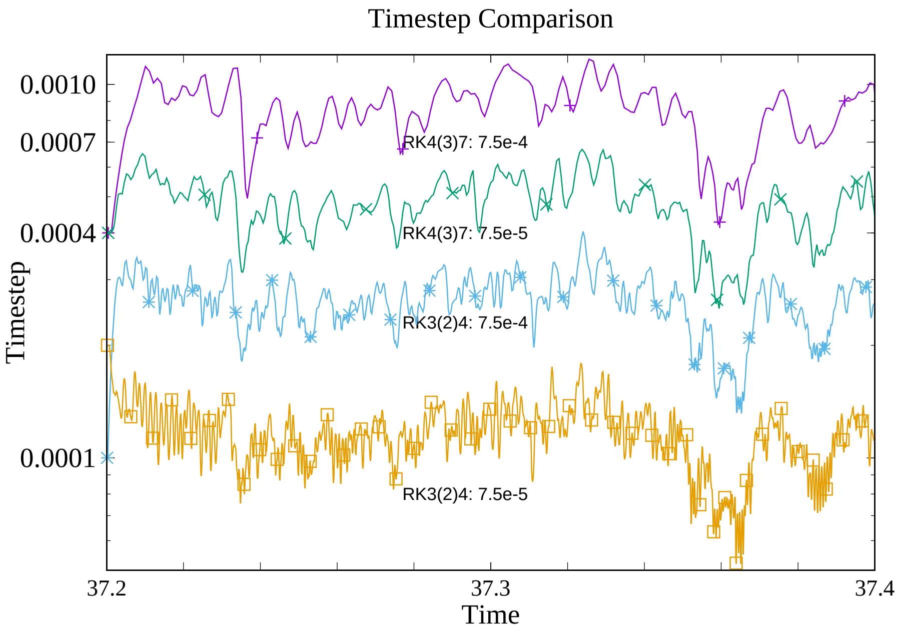
Efficacy of Solver Optimized Schemes

Head-to-Head Testing

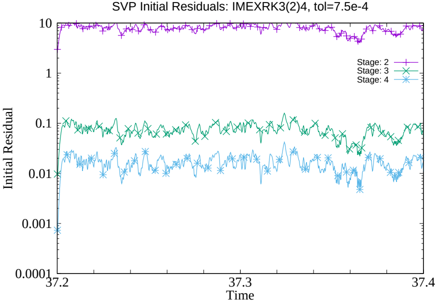
Which scheme is most efficient at large scale?

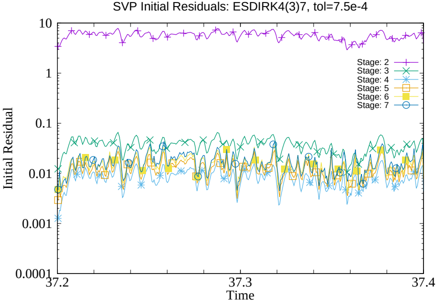
- Head-to-Head comparison
- SD7003: 116016 Hexahedral elements run at P3 and P4
- Test at Engineering error tolerances: e.g., tol $= 7.5\text{e-}5$ and $7.5\text{e-}4$ / timestep
- Test ONLY IMPLICIT operator from each IMEX pair
- Schemes:
  - IMEX3(2)4L[2]SA vs. IMEXRK4(3)7L[2]SA (KC: ANM 2003, 2019a)
  - IMEX3(2)4L[2]SA vs. ESDIRK4(3)7L[2]SA (KC: ANM 2003, 2019b)
  - IMEX4(3)6L[2]SA (KC: ANM, 2003)
  - IMEX5(4)8L[2]SA (KC: ANM, 2019b)

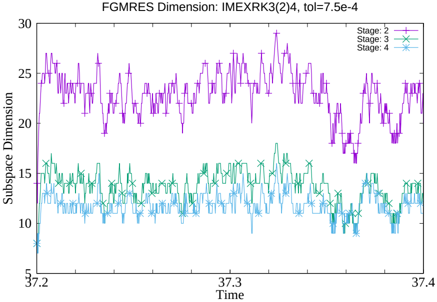
Physical Timestep Used By Schemes

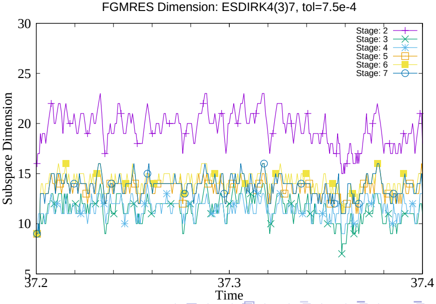


Convergence P3: IMEX324 vs. ESDIRK437

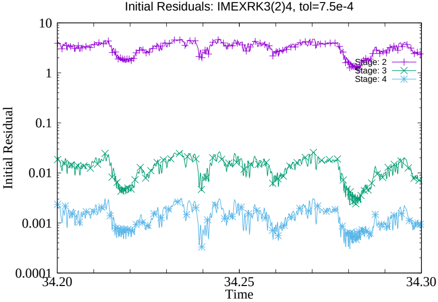


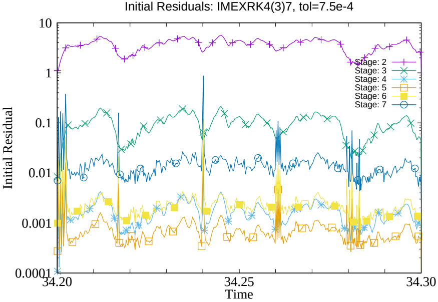


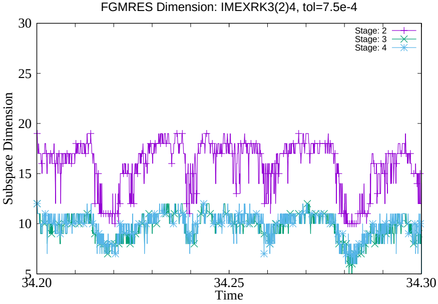


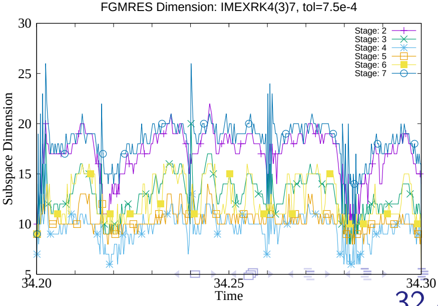


Convergence P4: IMEX324 vs. IMEXRK437









Efficacy of Solver Optimized Schemes: The Verdict is?

- Optimized schemes [RK4(3)7] are twice efficient than RK3(2)4
- Optimized schemes are more 1) accurate, 2) robust $\rightarrow$ 3) efficient

	P3: Tol=7.5e-5		P3: Tol=7.5e-4		P4: Tol=7.5e-4	
Method	*CPUTime*	*Steps*	*CPUTime*	*Steps*	*CPUTime*	*Steps*
*IMEXRK*3(2)4	61085	1792	68782	789	96694	1294
*IMEXRK*4(3)7	30076	434	34577	245	53318	328
*ESDIRK*4(3)7	35096	563	33799	314	61497	410
*ESDIRK*4(3)6	49439	664	64654	364		
*ESDIRK*5(4)8	42348	504	42523	297		

Discussion: Temporal Integrators

- Solver optimized schemes are the clear winner in these comparisons!
  - Comparisons were performed at fixed accuracy. (Not dt_{max})
- Additional stage: 1) more accurate ($\downarrow 10^2$) with 2) smaller γ ($\frac{1}{4} \rightarrow \frac{1}{8}$)
- Increased accuracy allows huge timesteps ($\uparrow 4$) relative to lower-order schemes.
- First cut for SVP is encouraging. Not yet where I want to be. (FGMRES 10-15/stage. $\rightarrow$, 3-5/stage)
- SVP and optimized γ enables equivalent iteration counts between 3^{rd}- and 4^{th}-order schemes
- Controllers achieved specified accuracy. Current focus: optimality

Thank You For Your Interest

Entropy Stability: an exciting eight years
More work needed on solvers and integrators

Thanks Nail for organizing Minisymposium
Hope you've enjoyed the talks!

Many thanks to all collaborators
and M. Malik (RCA-TTT) for support.