

Intrastep, Stage-Value Predictors for Diagonally-Implicit Runge–Kutta Methods

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Coworkers: And Many Special Thanks

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The View from 35,007'

Reliable Simulation Tools for Unsteady Phenomena

Technical Challenge: Develop robust and efficient 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)

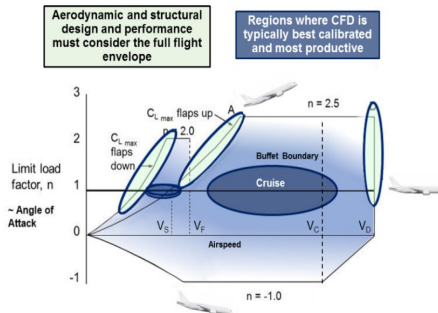


Figure: Load Factor/Airspeed Flight Envelope.

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 why a **stiff** Integrator?

- Sources of stiffness
 - ▶ 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
- Stiffness $\rightarrow$ Implicit methods (A-stability, L-stability)

An Ocean of Integrators; Married to Runge-Kutta

- Multipurpose integrator CFD: Linear Multistep, MultiStage, GLM
 - ▶ External Aero: nonstiff / stiff / separably stiff (IMEX, multirate)
 - ▶ Implicit RK: Stepwise & internal A- & L-stability → Robustness
 - ▶ Amenable to implicit/explicit partitioning → Efficiency
- Unique Algorithmic Constraints
 - ▶ HP-Adaptive Mesh Refinement → Self-starting → Runge-Kutta
 - ▶ Transmission stability conditions at refinement:
 - ▶ Our favorites: (E)SDIRK Runge-Kutta schemes
- Lessons learned with (E)SDIRK Schemes: Good news, Bad news
 - ▶ Extremely accurate. Factor 20 larger timestep (relative to BDF2)
 - ▶ H-O accuracy → multiple stages → mandates huge timesteps
 - ▶ Whack-a-mole: Increased burden on linear/nonlinear solver
- H-O spatial discretizations are notoriously difficult for solvers
 - ▶ DO NO HARM! Solver optimized (E)SDIRK schemes

Back to Ground Level

The Anatomy of a Stiff Integrator $\leftrightarrow$ Optimize Efficiency

- Entropy Stable discretization of NSE $\rightarrow$ O.D.E.
- The main integration scheme : $\mathbf{U}^n \rightarrow \mathbf{U}^{n+1}$
 - ▶ Implicit: Stepwise & internal A- & L-stability, (E)SDIRK
- 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 over-solve) Söderland
 - ▶ Reevaluate preconditioner Jacobian (only when needed)
 - ▶ $T_0 \rightarrow T_f$: Total cost = steps * $\frac{\text{stages}}{\text{step}}$ * $\frac{\text{cost}}{\text{stage}}$
- Solver: Linear/Nonlinear (big kahuna, $\dots$ weakest link for H-O DG)
 - ▶ Exact or approximate Jacobian Matrix
 - ▶ Factorization and storage of matrix
 - ▶ Nonlinear iteration loop (e.g., Newton's method)
 - ▶ Algebraic linear solver (e.g., GMRES)
- The components are intertwined! The “Whole Package” matters!

The Anatomy of a Stiff Integrator: Continued

- Solver Costs: What can be optimized?
 - ▶ Solver hardware optimization (obviously: [AVX512](#))
 - ▶ Algorithmic Choices ([ESDIRK](#) and [Newton](#))
 - ▶ Temporal: Second-order vs. high-order temporal scheme
 - ▶ Iterative: (Modified) Newton, Broyden, Anderson, ...
 - ▶ Hardware availability (conventional [CPU: Skylake](#))
 - ▶ 2 GB memory/core: Form approximate Jacobian, factorize and store
 - ▶ Reuse it forever! (20 Newton iterates; 300 Krylov vectors)
 - ▶ Amortizes cost of linear solve.
 - ▶ Dominant cost in our *stiff* integrator: nonlinear/linear solver
- GMRES cost; i.e., number of search directions
 - ▶ Temporal method [size of $\gamma \Delta t$; $(\mathbf{I} - \gamma \Delta t \mathbf{J})(\delta U_{i,k}) = -\mathbf{r}_{i,k}$]
 - ▶ Preconditioner: ILU(k), ILUT, ILUTP, Jacobi, Multigrid, DADI
 - ▶ Initial solution used to start nonlinear iteration: [SVPs](#)
- Starting solution is sensible place to begin optimization

Stage-Value Predictors (SVP)

A Quick Review: Stiffly Accurate ESDIRK schemes

Stiffly-accurate ($a_{sj} = b_j, j = 1, 2, \dots, s$), stage-order two methods

0	0	0	0	...	0	0	0
2γ	γ	γ	0	...	0	0	0
c_3	a_{31}	a_{32}	γ	$\ddots$	0	0	0
$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\ddots$	$\ddots$	$\vdots$	$\vdots$
c_{s-2}	$a_{s-2,1}$	$a_{s-2,2}$	$a_{s-2,3}$	$\ddots$	γ	0	0
c_{s-1}	$a_{s-1,1}$	$a_{s-1,2}$	$a_{s-1,3}$	...	$a_{s-1,s-1}$	γ	0
1	b_1	b_2	b_3	...	b_{s-1}	b_s	γ
	b_1	b_2	b_3	...	b_{s-2}	b_{s-1}	γ
	$\hat{b}_1$	$\hat{b}_2$	$\hat{b}_3$	...	$\hat{b}_{s-2}$	$\hat{b}_{s-1}$	$\hat{b}_s$

$\mathbf{A} = a_{ij}$, $\mathbf{b} = b_i$ and $\mathbf{c} = c_i$,

$$\begin{array}{c|c} \mathbf{c} & \mathbf{A} \\ \hline & \mathbf{b}^T \end{array} = \begin{array}{c|c} 0 & \mathbf{0}^T \\ \hline \hat{\mathbf{c}} & \hat{\mathbf{A}} \\ \hline & b_1 \hat{\mathbf{b}}^T \end{array} \quad \text{with} \quad \mathbf{A} = \begin{bmatrix} 0 & \mathbf{0}^T \\ a & \hat{\mathbf{A}} \end{bmatrix},$$

What are Stage-Value Predictors?

SVP design at stage k , the ESDIRK (left) and (EDIRK) right

0	0	0	...	0	0
2γ	γ	γ	...	0	0
c_3	a_{31}	a_{32}	$\ddots$	0	0
$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\ddots$	0
c_{k-1}	$a_{k-1,1}$	$a_{k-1,2}$	$\ddots$	γ	0
c_k	$a_{k,1}$	$a_{k,2}$	...	$a_{k,k-1}$	γ

$\mathbf{c} \mid \mathbf{A}$

0	0	0	...	0	0
2γ	γ	γ	...	0	0
c_3	a_{31}	a_{32}	$\ddots$	0	0
$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\ddots$	0
c_{k-1}	$a_{k-1,1}$	$a_{k-1,2}$	$\ddots$	γ	0
c_k	β_1	β_2	...	β_{k-1}	0

$\mathbf{c} \mid \tilde{\mathbf{A}}$

The SVP for stage k is implemented as

$$U_{k,0} = U^{[n]} + (\Delta t) \sum_{j=1}^{k-1} \beta_{kj} F_j,$$

where $U_{k,0}$ is the approximation to U_k .

A Brief History: Stage-Value Predictors (SVPs)

- Sand, Hairer & Wanner, Laburta, Higueras & Roldán, Roldán, González-Pinto, Calvo, Olsson & Söderland, Skvortsov ...
 - ▶ Sand (1988,1992) Derived order and inverse order conditions
 - ▶ Laburta (1997,1998,1999) Additional function evaluations
 - ▶ Hairer Lubich, & Wanner extend Laburta's work (2006)
 - ▶ Higueras and Roldán (1999,2000,2002,2003,2004,2005)
 - ▶ Multistep SVP for IRK and (E)SDIRKs
 - ▶ RK schemes for DAE-I,
 - ▶ Order conditions for DAE-II
 - ▶ González-Pinto (2000,2001,2003)
 - ▶ Type I: solution SVP vs. Type II: solution+function
 - ▶ Nonstiff and stiff order conditions, Order reduction
 - ▶ Stiff components must be treated with *stable SVPs*
 - ▶ Calvo and Portillo (2003,2005) Low-order can outperform high order
 - ▶ A delicate balance of accuracy and stability constraints
- SVP: Long History in RK literature (NASATM:219173)

Stage-Value Predictors: Continued

- The Role of SVPs
 - ▶ Starting Newton iterate inside quadratic convergence ball
 - ▶ Reduces *meandering* convergence at startup
 - ▶ Fewer nonlinear iterates needed to achieve convergence
 - ▶ Typical convergence in 2-3 nonlinear iterates
 - ▶ Affects convergence rate of *linear solver*
 - ▶ Not all $\|\mathbf{r}\| = 10^{(-2)}$ are created equally
 - ▶ Not an issue with direct solvers (e.g., Kap's, Van der Pol's)
- Accuracy of SVP: Y_i^0 relative to converged stage Y_i
 - ▶ $|Y_i - Y_i^0| = O(h^{p+1})$, Differential variable
 - ▶ $|Y_i - Y_i^0| = O(h^{q+1})$, Algebraic variable (stiff component)
- Conventional Wisdom for constructing SVPs
 - ▶ High-order SVPs for tight error tolerances (e.g. 10^{-7}):
 - ▶ Low-order SVPs for coarse error tolerances (e.g. 10^{-3}):
 - ▶ Switching mechanics for choosing appropriate SVP

Design Considerations: Stage Order Conditions

Stage order-conditions up to fifth-order for Runge–Kutta methods.

$t_1^{(1)}$	$\mathbf{Ae} - \frac{\mathbf{c}}{1!}$	$t_1^{(2)}$	$\mathbf{Ac} - \frac{\mathbf{c}^2}{2!}$
$t_1^{(3)}$	$\frac{1}{2!}\mathbf{Ac}^2 - \frac{\mathbf{c}^3}{3!}$	$t_2^{(3)}$	$\mathbf{AAc} - \frac{\mathbf{c}^3}{3!}$
$t_1^{(4)}$	$\frac{1}{3!}\mathbf{Ac}^3 - \frac{\mathbf{c}^4}{4!}$	$t_2^{(4)}$	$\mathbf{ACA} - \frac{3\mathbf{c}^4}{4!}$
$t_3^{(4)}$	$\frac{1}{2!}\mathbf{AAc}^2 - \frac{\mathbf{c}^4}{4!}$	$t_4^{(4)}$	$\mathbf{AAA} - \frac{\mathbf{c}^4}{4!}$
$t_1^{(5)}$	$\frac{1}{4!}\mathbf{Ac}^4 - \frac{\mathbf{c}^5}{5!}$	$t_2^{(5)}$	$\frac{1}{2!}\mathbf{Ac}^2\mathbf{Ac} - \frac{6\mathbf{c}^5}{5!}$
$t_3^{(5)}$	$\frac{1}{2!}\mathbf{A}(\mathbf{Ac})^2 - \frac{3\mathbf{c}^5}{5!}$	$t_4^{(5)}$	$\frac{1}{2!}\mathbf{ACA} - \frac{4\mathbf{c}^5}{5!}$
$t_5^{(5)}$	$\frac{1}{3!}\mathbf{AAc}^3 - \frac{\mathbf{c}^5}{5!}$	$t_6^{(5)}$	$\mathbf{ACA} - \frac{4\mathbf{c}^5}{5!}$
$t_7^{(5)}$	$\mathbf{AACAc} - \frac{3\mathbf{c}^5}{5!}$	$t_8^{(5)}$	$\frac{1}{2!}\mathbf{AAA} - \frac{\mathbf{c}^5}{5!}$
$t_9^{(5)}$	$\mathbf{AAAA} - \frac{\mathbf{c}^5}{5!}$		

$$\underline{\mathbf{c}} \mid \mathbf{A}$$

$$\Delta t_1^{(1)} = t_1^{(1)} - \tilde{t}_1^{(1)},$$

$$\underline{\mathbf{c}} \mid \tilde{\mathbf{A}}$$

$$A_i^{(p+1)} = \|t_i^{(p+1)}\|_2 = \sqrt{\sum_{j=1}^{a_{p+1}} \left(t_{j,i}^{(p+1)}\right)^2} \quad ; \quad \Delta A_i^{(p+1)} = \sqrt{\sum_{j=1}^{a_{p+1}} \left(\Delta t_{j,i}^{(p+1)}\right)^2}.$$

Design Considerations: Internal Stability

Baseline and SVP stability functions

$$\begin{aligned}R_{\text{int}(z)}^b &= (\mathbf{I} - z\mathbf{A})^{-1}\mathbf{e} \\R_{\text{int}(z)} &= (\mathbf{I} - z\tilde{\mathbf{A}})^{-1}\mathbf{e} = \{R_{\text{int}}^{(1)}(z), R_{\text{int}}^{(2)}(z), \dots, R_{\text{int}}^{(s)}(z)\}^T \\&= \left\{ \frac{P_{\text{int}}^{(1)}(z)}{Q_{\text{int}}^{(1)}(z)}, \frac{P_{\text{int}}^{(2)}(z)}{Q_{\text{int}}^{(2)}(z)}, \dots, \frac{P_{\text{int}}^{(s)}(z)}{Q_{\text{int}}^{(s)}(z)} \right\}^T.\end{aligned}$$

E-polynomial at internal stages is used to determine stagewise l-stability

$$E_{\text{int}}^{(i)}(y) = Q_{\text{int}}^{(i)}(iy)Q_{\text{int}}^{(i)}(-iy) - P_{\text{int}}^{(i)}(iy)P_{\text{int}}^{(i)}(-iy),$$

where $E_{\text{int}}^{(i)}(y) \geq 0$, $y \geq 0$ implies stagewise l-stability.

Stagewise analog to internal algebraic-stability matrix: $M_{jk}^{(i)}$ for stage i .

$$M_{jk}^{(i)} = \tilde{a}_{ij}\tilde{a}_{jk} + \tilde{a}_{ik}\tilde{a}_{kj} - \tilde{a}_{ij}\tilde{a}_{ik} \geq 0, \quad \tilde{a}_{ij} \geq 0, \quad i, j, k = 1, 2, \dots, s,$$

- Base Scheme: Better base scheme $\rightarrow$ better SVPs
 - ▶ 1) Stepwise A- and L-stability with stiff accuracy, 2) stage order two, 3) stagewise A-stability, and L-stability (if possible), 4) minimize stage and stepwise algebraic instability
- Stage-value predictor definitions (for sequential SDIRK schemes)
 - ▶ Intrastep: Using only data within the current step
 - ▶ Interstep: Using current and previous timestep data
- What to enforce? Stage k : intrastep predictor has $k - 1$ (DoFs).
 - ▶ Enforce order conditions $\Delta t_1^{(1)} \dots \Delta t_2^{(4)} \quad (1, 2, 3, 4 \rightarrow 1, 1, 1, 2)$
 - ▶ Enforce stability conditions
 - ▶ Reduce Order of stability polynomial $\beta_1 = \beta_2$
 - ▶ Enforce damping at $-\infty$: $R(-\infty) = 0$
 - ▶ Enforce linear stability: Stagewise A-stability (not guaranteed) and L-stability if possible
 - ▶ Enforce nonlinear order conditions: minimize ?
 - ▶ Minimize size of coefficients ?

- SVP design study: two distinct ESDIRKs (contributes to generality)
 - ▶ Existing: ESDIRK4(3)7L[2]SA, $\gamma = 1/8$
 - ▶ New : ESDIRK4(3)8L[2]SA, $\gamma \approx 1/10$

Scheme	1	2	3	4	5	6	7	8
ESDIRK4(3)7L[2]SA	0	0.250	0.0732	0.500	0.696	0.706	1	
ESDIRK4(3)8L[2]SA	0	0.201	0.0590	0.414	0.569	0.773	0.742	1

Table: Abscissae for ESDIRK schemes.

- ▶ Build SVPs for each stage using different design objectives
 - ▶ Early stages: Limited constraints
 - ▶ Later stages: (≥ 5): Build multitude of A-stable SVPs
 - ▶ Compare efficacy of accuracy and stability designs
 - ▶ Build SVPs with one bad design metric (e.g., $\|\mathcal{M}\|$)
 - ▶ Over weighting recent stage data
 - ▶ Minimize $\|\beta_j\|$

Test Problems and Solver Mechanics

Test Problems: SD7003 and MD30P30N airfoils

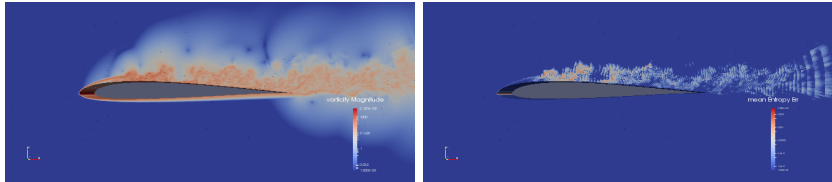


Figure: Vorticity magnitude and spatial error estimate

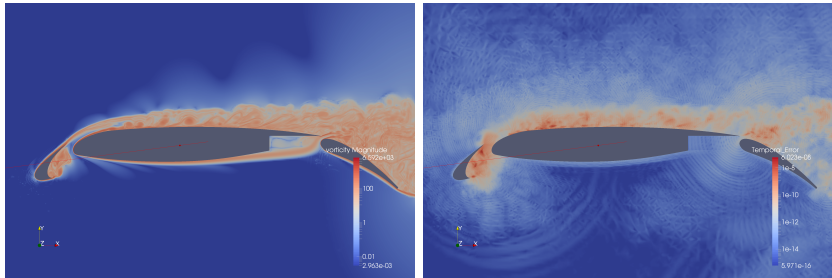


Figure: Vorticity magnitude and temporal error estimate

- Two large scale 3D airfoil problems
- Unstructured curvilinearly mapped hex elements. $\approx 10^4 - 10^5$ elements
- Entropy Stable-Spectral collocation.
 - ▶ BCs: 1) free stream farfield, 2) SS Solid Wall, 3) Periodic
 - ▶ Polynomial orders P3 and P5 (fourth- and sixth-order)
- PID-H321 controller adjusts timestep over interval $40.0 \leq T \leq 40.25$
 - ▶ Step-size control was on L_{infty} error.
 - ▶ Target errors in range $10^{-2} - 10^{-5}$ / step
 - ▶ L_{infty} error was approximately 10x error in integrated quantities (e.g., Lift, Drag)

	SD7003 Airfoil		30P30N multielement	
poly	D.O.F.	dt_{explct}	D.O.F.	dt_{explct}
1	0.45×10^6	1.4×10^{-5}	0.12×10^7	5.6×10^{-5}
2	1.50×10^6	3.0×10^{-6}	0.42×10^7	1.5×10^{-5}
3	3.60×10^6	1.0×10^{-6}	1.00×10^7	4.8×10^{-6}
4	7.09×10^6	5.8×10^{-7}	1.95×10^7	2.5×10^{-6}
5	12.2×10^6	3.3×10^{-7}	3.37×10^7	1.6×10^{-6}
6	19.4×10^6	1.8×10^{-7}	5.35×10^7	7.5×10^{-7}

Table: Grid stiffness and D.O.F. for the SD7003 and 30P30N FEM meshes.

A common definition of stiffness: $\frac{\Delta t_{physics}}{\Delta t_{explicitCFL}}$

$$SD7003 : \frac{3.5 \times 10^{-3}}{3.3 \times 10^{-7}} \approx 10^4 \quad ; \quad 30P30N : \frac{1.5 \times 10^{-4}}{1.5 \times 10^{-6}} \approx 10^2$$

Solvers: Another talk for another day!

- Conventional Architecture: 2.0GB/process
 - ▶ Enables storing factored preconditioner
- Solver Mechanics: infrastructure
 - ▶ (JacFree) Newton-Krylov, Preconditioned with “Reduced-Jacobian”
 - ▶ Classical Dom-Decomp: Additive-Schwarz (1 layer overlap)
 - ▶ Preconditioned GMRES
 - ▶ Approximate Preconditioning matrix: Thin-layer NS
 - ▶ Preconditioner: ILUTP, $T = 10^{-2}$, $L_{fil} = 16$
 - ▶ Stored ILU factors: 20 Newton Iterations
 - ▶ Arnoldi subspace $AP P^{-1} V^n = \bar{V}^{n+1} \bar{H}$ using Frechet derivatives
 - ▶ Newton Update
 - ▶ Trust-Region / line search
 - ▶ Stage-value predictor used at beginning of each RK stage

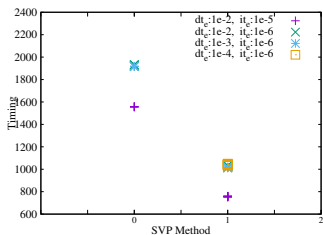
Controllers: Another talk for another day!

- Error Estimators $||\epsilon|| = ||\mathbf{U}^{n+1} - \hat{\mathbf{U}}^{n+1}||$
- Controller (NASATM:219173)
 - ▶ Söderland's PPID
$$(\Delta t)^{[n+1]} = \kappa (\Delta t)^{[n]} \left\{ \frac{\text{tol}}{||\epsilon^{[n+1]}||} \right\}^{\alpha} \left\{ \frac{||\epsilon^{[n+0]}||}{\text{tol}} \right\}^{\beta} \left\{ \frac{\text{tol}}{||\epsilon^{[n-1]}||} \right\}^{\delta} \left\{ \frac{(\Delta t)^{[n]}}{(\Delta t)^{[n-1]}} \right\}$$
$$\alpha = +\frac{0.30}{\hat{\rho}}, \beta = -\frac{0.05}{\hat{\rho}}, \delta = -\frac{0.25}{\hat{\rho}}, \text{tol} = \text{user input}$$
 - ▶ Tolerance (tol) set to 7.5e-4, 7.5e-5 in L_{∞}
 - ▶ Used for all tests with NO TUNING: “HANDS-OFF”

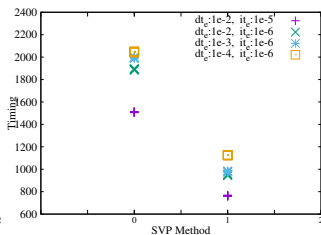
Results

- Testing ESDIRK4(3)7L[2]SA and ESDIRK4(3)7L[2]SA
- Plots of SVP stage timings and Table of SVP design attributes
- Plots
 - ▶ Four (for P3) distinct test cases varying: (two for P5)
 - ▶ *controller error targets: dt_e*
 - ▶ *nonlinear iteration tolerances: it_e*
 - ▶ Trivial guess timing: *method 0*
 - ▶ Coarsest tolerances are preferentially treated $dt_e:1e-2, it_e:1e-5$.
- Tables
 - ▶ Column denoted *Design* provides the design objectives
 - ▶ 1,2,3,4a,4b $\rightarrow \Delta t_1^{(1)}, \Delta t_1^{(2)}, \Delta t_1^{(3)}, \Delta t_1^{(4)}, \Delta t_2^{(4)}$, respectively.
 - ▶ A, L, M $\rightarrow$ stability properties
A-stability, L-stability algebraic instability: $\|\mathcal{M}\|$

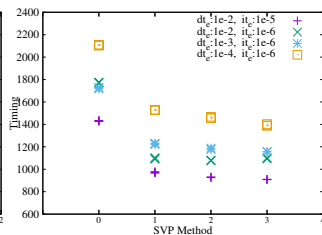
SVP Timings: ESDIRK4(3)7L[2]SA



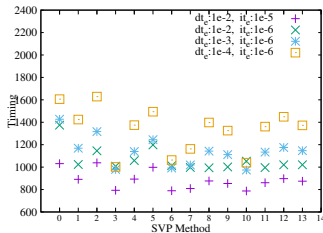
(a) P3: Stage 3



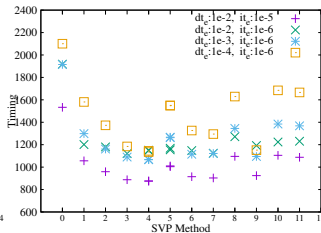
(b) P3: Stage 4



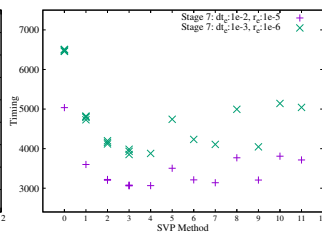
(c) P3: Stage 5



(d) P3: Stage 6



(e) P3: Stage 7



(f) P5: Stage 7

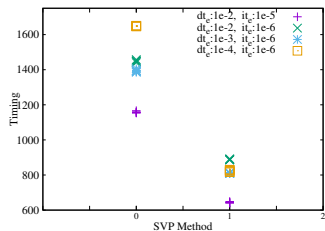
Figure: ESDIRK4(3)7L[2]SA Timings

SVP Design Properties: ESDIRK4(3)7L[2]SA

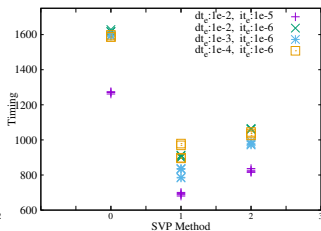
SVP	Design	A_{stab}	L_{stab}	$R(-\infty)$	$-\ \mathcal{M}\ $	$\ \beta\ $	$\ \Delta A^{(2)}\ $	$\ \Delta A^{(3)}\ $	$\ \Delta A^{(4)}\ $
3.1	1	Y	N	0.4142	-0.0023	0.30	0.0065	0.0027	0.0043
SVP	Design	A_{stab}	L_{stab}	$R(-\infty)$	$-\ \mathcal{M}\ $	$\ \beta\ $	$\ \Delta A^{(3)}\ $	$\ \Delta A^{(4)}\ $	$\ \Delta A^{(5)}\ $
4.1	A N	Y	N	1.0	-3.0261	0.85	0.0027	0.0043	0.0023
5.1	3	N	N	-2.829	-31.613	2.53	0.0	0.0062	0.0019
5.2	A3	Y	N	-0.992	-12.217	1.58	0.0051	0.0032	0.0033
5.3	AL	Y	n	-0.056	-5.891	1.09	0.0077	0.0066	0.0053
6.1	34	N	N	-0.004	-0.354	0.162	0.0	0.0011	0.0013
6.2	3M	N	N	+3.137	-28.04	2.156	0.0	0.0068	0.0025
6.3	3B	N	N	-1.601	-5.591	0.987	0.0	0.0038	0.0016
6.4	A3	Y	N	1.000	-0.739	0.318	0.0067	0.0082	0.0061
6.5	AM	Y	N	-1.000	-18.256	1.754	0.0170	0.0150	0.0130
6.6	A3	Y	N	-0.997	-4.867	0.918	0.0049	0.0042	0.0044
6.7	AL	Y	Y	0.0	-0.603	0.333	0.0058	0.0058	0.0051
6.8	AL	Y	Y	0.0	-0.244	0.142	0.0016	0.0022	0.0023
6.9	AL	Y	N	-0.202	-0.255	0.210	0.0016	0.0021	0.0022
6.10	AL	Y	n	10^{-10}	-2.007	0.587	0.0098	0.0093	0.0079
6.11	AL	Y	n	10^{-6}	-0.234	0.147	0.0020	0.0025	0.0025
6.12	3L	N	N	0.0	-0.357	0.164	0.0	0.0011	0.0013
6.13	3L	N	N	0.274	-0.241	0.177	0.0	0.0013	0.0013
7.1	34ab	N	N	-1.617	-62.54	3.008	0.0	0.0	0.0097
7.2	34a	N	N	-3.837	-130.66	4.336	0.0	0.0048	0.0082
7.3	34b	N	N	-1.618	-62.91	3.02	0.0	0.0003	0.0098
7.4	3M	N	N	-2.331	-1.64	0.524	0.0	0.0110	0.0120
7.5	A	Y	N	1.000	-5.51	0.937	0.0074	0.0073	0.0094
7.6	A	Y	N	-1.000	-26.24	1.957	0.0095	0.0110	0.0010
7.7	AL	Y	n	10^{-7}	-12.96	1.389	0.0092	0.0097	0.0099
7.8	M	N	N	1.022	-0.73	0.340	0.0190	0.0220	0.0200
7.9	ALM	Y	Y	0.0	-0.85	0.358	0.0290	0.0290	0.0220
7.10	3	N	N	1.800	-6.00	0.990	0.0	0.0075	0.0120
7.11	3	N	N	0.0	-28.68	2.050	0.0	0.0035	0.0120

Table: SVP properties for stages three to seven.

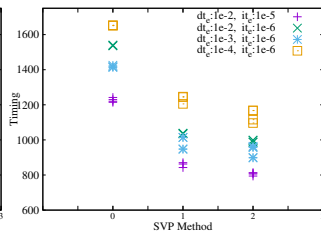
SVP Timings: ESDIRK4(3)8L[2]SA



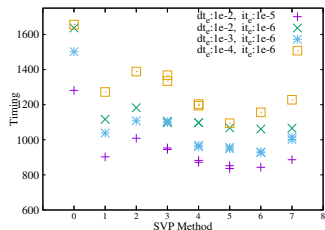
(a) Stage 3



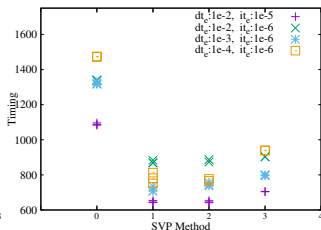
(b) Stage 4



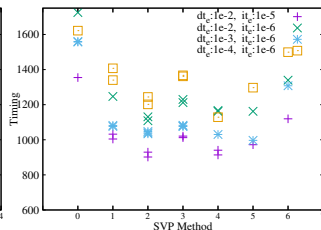
(c) Stage 5



(d) Stage 6



(e) Stage 7



(f) Stage 8

Figure

SVP Design Properties: ESDIRK4(3)8L[2]SA

SVP	Design	A_{stab}	L_{stab}	$R(-\infty)$	$-\ \mathcal{M}\ $	$\ \beta\ $	$\ \Delta A^{(2)}\ $	$\ \Delta A^{(3)}\ $	$\ \Delta A^{(4)}\ $
3.1	A 1	Y	N	0.4142	-0.0023	0.24	0.0042	0.0012	0.00027
4.1	A 2	N	N	1.21	-2.2629	0.74	0.0	0.0017	0.0021
4.2	A L	N	N	0.0	-1.2990	0.85	0.012	0.0043	0.0023
SVP	Design	A_{stab}	L_{stab}	$R(-\infty)$	$-\ \mathcal{M}\ $	$\ \beta\ $	$\ \Delta A^{(3)}\ $	$\ \Delta A^{(4)}\ $	$\ \Delta A^{(5)}\ $
5.1	3	N	N	-3.408	-15.611	1.78	0.0	0.0021	0.00057
5.2	AL	Y	N	-0.191	-2.071	0.64	0.0051	0.0032	0.0033
6.1	3	N	N	-0.537	-9.403	1.28	0.0	0.0014	0.0032
6.2	3	N	N	+9.993	-31.830	2.29	0.0	0.0056	0.0038
6.3	3	N	N	+3.891	-0.615	0.29	0.0	0.0021	0.0033
6.4	L3	N	N	+0.000	-12.637	1.47	0.0	0.0014	0.0032
6.5	AL	Y	N	+0.16	-14.05	1.55	0.0045	0.0043	0.0054
6.6	A3	Y	N	+0.729	-9.992	1.31	0.0036	0.0039	0.0050
6.7	AM	Y	N	+0.999	-8.699	1.23	0.0040	0.0043	0.0052
7.1	A34	Y	N	0.027	-4.434	0.811	0.0	0.0	0.0032
7.2	A3L	Y	Y	0.000	-4.441	0.812	0.0	1×10^{-5}	0.0038
7.3	A3LM	Y	Y	0.000	-0.329	0.207	0.0	5×10^{-4}	0.0073
8.1	M3	N	N	0.00	-1.17	0.415	0.0	0.0140	0.0021
8.2	AN	Y	N	-1.00	-43.17	3.415	0.0014	0.0140	0.0052
8.3	M	N	N	+1.00	-2.47	0.415	0.0013	0.0140	0.0031
8.4	AL	Y	Y	+0.0	-53.17	2.569	0.0100	0.010	0.0017
8.5	AL	Y	Y	+0.00	-26.17	1.807	0.0069	0.0120	0.0003
8.6	34	N	N	+25.0	-4.32	0.805	0.0	0.0	0.0038

Table: SVP properties for stages three to eight.

- SVP for ESDIRK4(3)7L[2]SA and ESDIRK4(3)7L[2]SA are tested
- *Nearly all SVPs outperform trivial guess*
- Groups of equally performant SVPs emerged on the later stages
 - ▶ 6, 7 for ESDIRK4(3)7L[2]SA and 6, 8 for ESDIRK4(3)8L[2]SA.
 - ▶ One or more SVPs is 1) A-stable, and fully or partially 2) L-stable on every stage
- Hierarchy of design constraints
 - 1) $\Delta t_1^{(1)} = 0$,
 - 2) $\beta_1 - \beta_2 = 0$,
 - 3) $\Delta t_1^{(2)} = 0$,
 - 4) A-stability,
 - 5) L-stability,
 - 6) $\Delta t_1^{(3)} = 0$,
 - 7) $\|\mathcal{M}\|$ (or minimize $\|\beta_j\|$),
 - 8) $\Delta t_1^{(4)} = \Delta t_2^{(4)} = 0$.
- Open questions
 - ▶ A-stability vs. $\Delta t_1^{(3)} = 0$?
 - ▶ Neutrally A-stable performs well?
 - ▶ $\Delta t_1^{(3)} = 0$ usually bad, but sometimes not ?

Relative Efficiency of ESDIRK Schemes

Efficiency Landscape for ESDIRK Schemes

- Comparison of six ESDIRK schemes
 - ▶ P3 with 11K hex elements on SD7003 airfoil
 - ▶ Optimal predictors for two current schemes
 - ▶ Accuracy based predictors for all other schemes
 - ▶ PID-H321 Controller

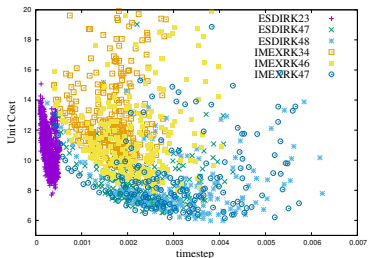
Time Error	$dt_e = \epsilon_{target} = 10^{-2}$			$dt_e = \epsilon_{target} = 10^{-4}$			$dt_e = \epsilon_{target} = 10^{-6}$		
Nonlin resid	$it_e = \epsilon_{resid} = 10^{-5}$			$it_e = \epsilon_{resid} = 10^{-6}$			$it_e = \epsilon_{resid} = 10^{-8}$		
Scheme	SVP	Trivial	η	SVP	Trivial	η	SVP	Trivial	η
ESDIRK23	16310	19933	0.81	52058	61608	0.84	382780	-	-
ESDIRK47	12048	17392	0.69	17130	25648	0.66	32195	57466	0.56
ESDIRK48	12058	17594	0.68	16009	23829	0.67	29642	55737	0.53
IMEXRK34	20693	25189	0.82	29941	44539	0.67	71655	108195	0.66
IMEXRK46	18133	27548	0.65	22299	36692	0.60	43928	82467	0.53
IMEXRK47	12637	18667	0.67	15155	24199	0.62	29961	56064	0.53

Table: Timings for three target errors ϵ_t

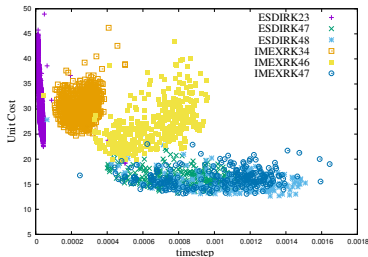
- Winners: fourth-order and seven or eight stages
- Same results at all level levels

Fine Grain Comparison of cost.

Scatter plots

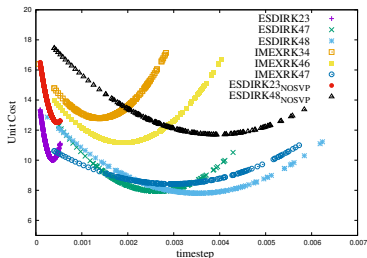


(a) $dt_e = 10^{-2}, it_e = 10^{-5}$

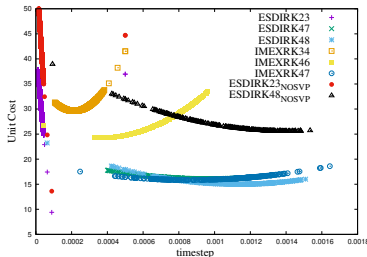


(c) $dt_e = 10^{-4}, it_e = 10^{-6}$

Cubic Fit



(b) $dt_e = 10^{-2}, it_e = 10^{-5}$



(d) $dt_e = 10^{-4}, it_e = 10^{-6}$

Conclusions

- Investigation to assess necessary attributes of good SVPs is performed
- Existing: ESDIRK4(3)7L[2]SA & new: ESDIRK4(3)8L[2]SA scheme
- ≤ 13 SVPs constructed for all stages with varying design objectives
- Trade studies are made between
 - 1) accuracy, 2) linear stability, 3) nonlinear stability
- All tested on aerofoil simulations (10^7 DoFs) using NSE
- Simulations performed at a wide variety of temporal error tolerances
- At lax temporal error tolerances, $\rightarrow$ enforce multiple stability properties: A- and L-stability, nonlinear stability
- Simulations at tight error tolerances, $\rightarrow$ enforce high accuracy
- One SVP stage: 4th-order, A- and nearly L-stable, Best performer with 100% improvement over trivial guess (60 – 70% combined step)
- Two aforementioned schemes are compared with four other ESDIRKs
- Best performing scheme across all error tolerances:
ESDIRK4(3)8L[2]SA scheme with $\gamma \approx 1/10$

Thank You For Your Interest

Many thanks to all collaborators
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