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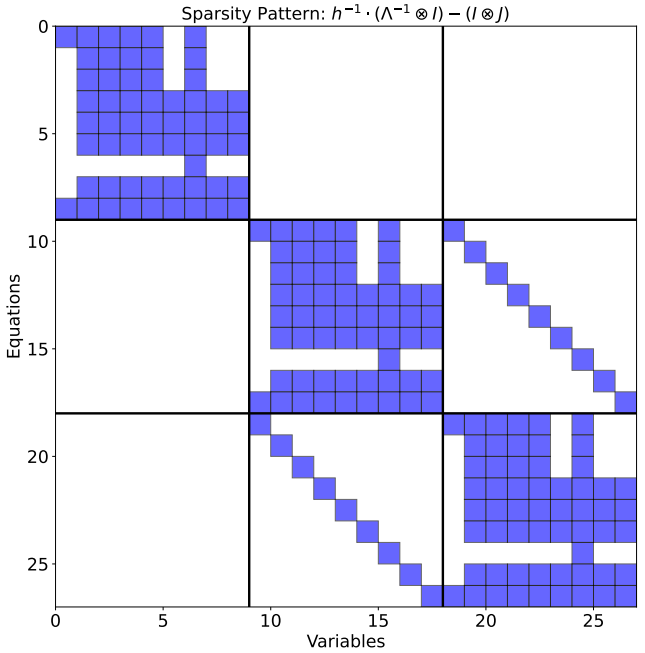

Advancements in Numerical Methods for the GBODE Solver

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GBODE

- Generic Bi-Rate Ordinary Differential Equation Solver - $\dot{\boldsymbol{y}}(t) = \boldsymbol{f}(t, \boldsymbol{y})$
- Implementation supports a wide range of Runge-Kutta methods
  - → Implicit: ESDIRK, SDIRK, Lobatto, Radau, Gauss, ...
  - → Explicit: Fehlberg, Merson, DOPRI45, ...
- Arising nonlinear systems of implicit methods are solved with KINSOL
- Special structure and context of the NLS is not used to full extend
  - → Convergence and speed can be improved by exploiting the structure of the NLS
  - → Strategies are implemented in the new flag `-gbnls=internal`

RUNGE-KUTTA METHODS

- Runge-Kutta methods compute several stage slopes

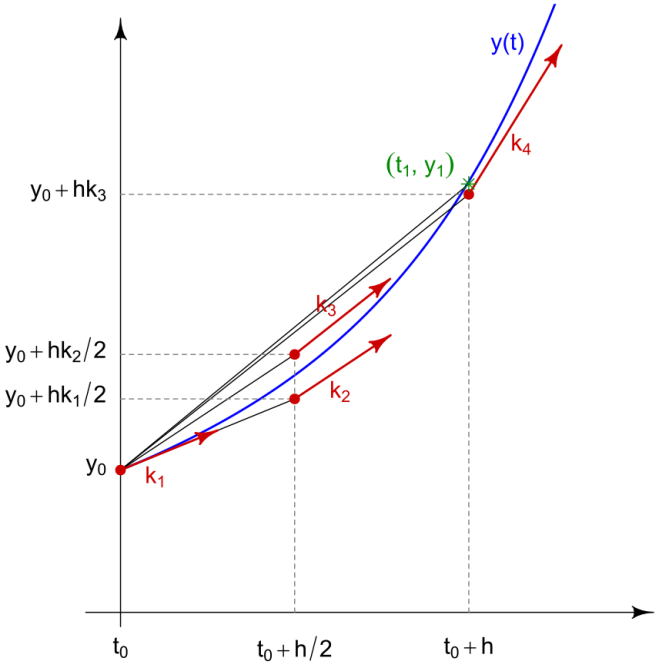
$$\boldsymbol{k}_i = \boldsymbol{f}\left(t_k + c_i h,\ \boldsymbol{y}_k + h \sum_{j=1}^{s} a_{ij} \boldsymbol{k}_j \right), \qquad i = 1, \dots, s$$

- These stage slopes are combined to update the solution

$$\boldsymbol{y}_{k+1} = \boldsymbol{y}_k + h \sum_{i=1}^{s} b_i \boldsymbol{k}_i$$

- The method coefficients are summarized in the Butcher tableau:

$$\begin{array}{c|ccc} c_1 & a_{11} & \cdots & a_{1s} \\ \vdots & \vdots & & \vdots \\ c_s & a_{s1} & \cdots & a_{ss} \\ \hline & b_1 & \cdots & b_s \end{array}$$



CLASSES OF IMPLICIT RUNGE-KUTTA METHODS

Singly Diagonal Implicit Runge-Kutta (ESDIRK / SDIRK)

$$\begin{array}{c|cccc} \gamma & \gamma & 0 & \cdots & 0 \\ c_2 & a_{21} & \gamma & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & 0 \\ c_s & a_{s1} & \cdots & a_{s,s-1} & \gamma \\ \hline & b_1 & b_2 & \cdots & b_s \end{array}$$

- Stages solved sequentially ($n \times n$ systems)
- Single diagonal parameter γ
- Uses a single LU factorization - $\mathcal{O}(n^3)$
- Efficient Newton iterations
- A- / L-stable schemes available

Fully Implicit Runge-Kutta (FIRK)

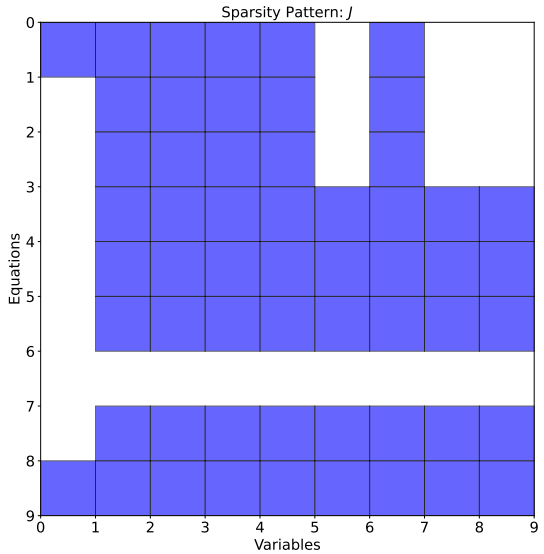
$$\begin{array}{c|cccc} c_1 & a_{11} & a_{12} & \cdots & a_{1s} \\ c_2 & a_{21} & a_{22} & \cdots & a_{2s} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ c_s & a_{s1} & a_{s2} & \cdots & a_{ss} \\ \hline & b_1 & b_2 & \cdots & b_s \end{array}$$

- Fully coupled stages
- Solve one $sn \times sn$ system - $\mathcal{O}\left((sn)^3\right)$
- Higher achievable order
- Excellent stability properties
- Seems to be very expensive compared to SDIRK methods

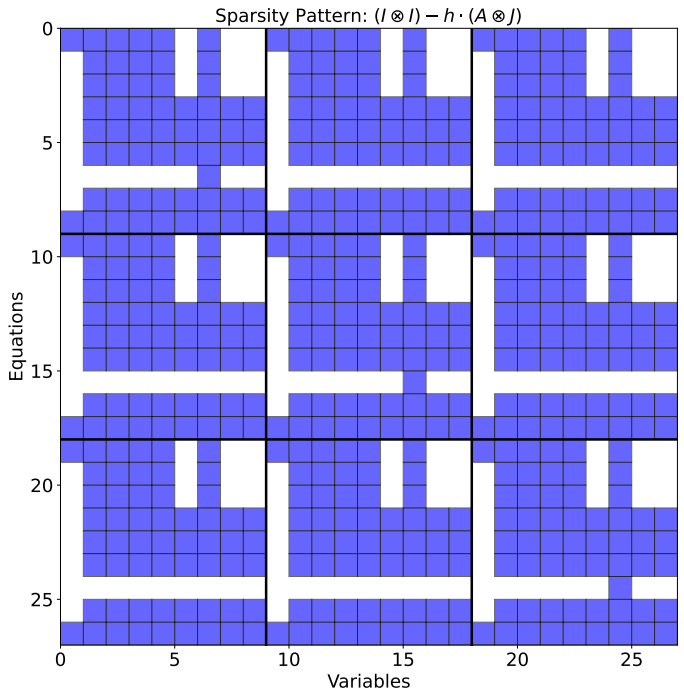
→ How to make this efficient?

EFFICIENT NLS FOR FIRK

- In the next few slides we will apply a series of transformations to the naive nonlinear system
- The visualizations and example matrices are for the specific 3-step Radau IIA method
- The theory is implemented for all FIRK methods in GBODE (incl. singular Butcher matrices)
- Consider the ODE sparsity pattern:



EFFICIENT NLS FOR FIRK: NAIVE / K-SPACE FORMULATION



Nonlinear System

$$\boldsymbol{g}_i(\boldsymbol{K}) := \boldsymbol{k}_i - \boldsymbol{f}\left(t_k + c_i h,\ \boldsymbol{y}_k + h \sum_{j=1}^{s} a_{ij} \boldsymbol{k}_j\right) = \boldsymbol{0}$$

Block-Jacobian

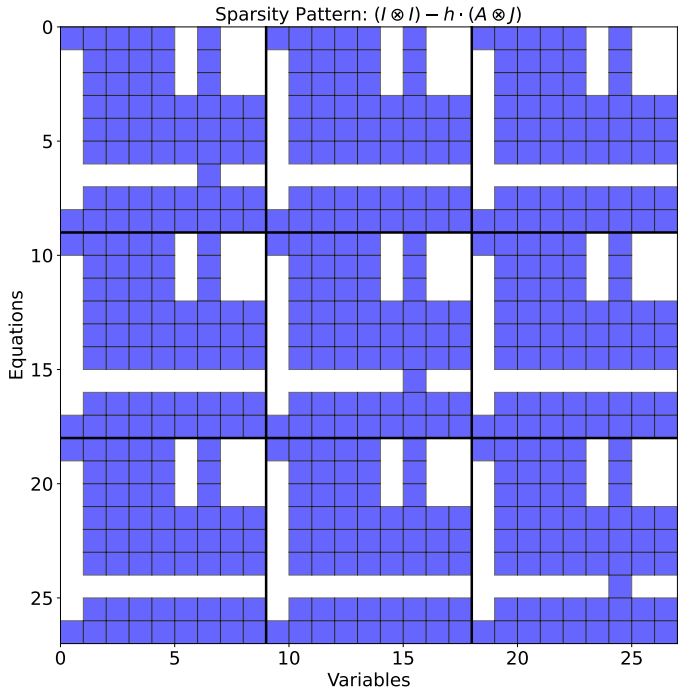
$$\frac{\partial \boldsymbol{g}_i}{\partial \boldsymbol{k}_j} = \delta_{ij} I_n - h\, a_{ij}\, J, \qquad J := \frac{\partial \boldsymbol{f}}{\partial \boldsymbol{y}}(t_0, \boldsymbol{y}_0)$$

Nonlinear System Jacobian

$$\frac{\partial \boldsymbol{G}_K}{\partial \boldsymbol{K}} = I_s \otimes I_n - h\, A \otimes J$$

→ LU factorization is $\mathcal{O}((sn)^3)$, here $\mathcal{O}(27n^3)$

EFFICIENT NLS FOR FIRK: Z-SPACE FORMULATION



Variable Transformation (assuming $\det A \neq 0$)

$$\boldsymbol{Z} := h(A \otimes I_n)\boldsymbol{K}$$

Nonlinear System

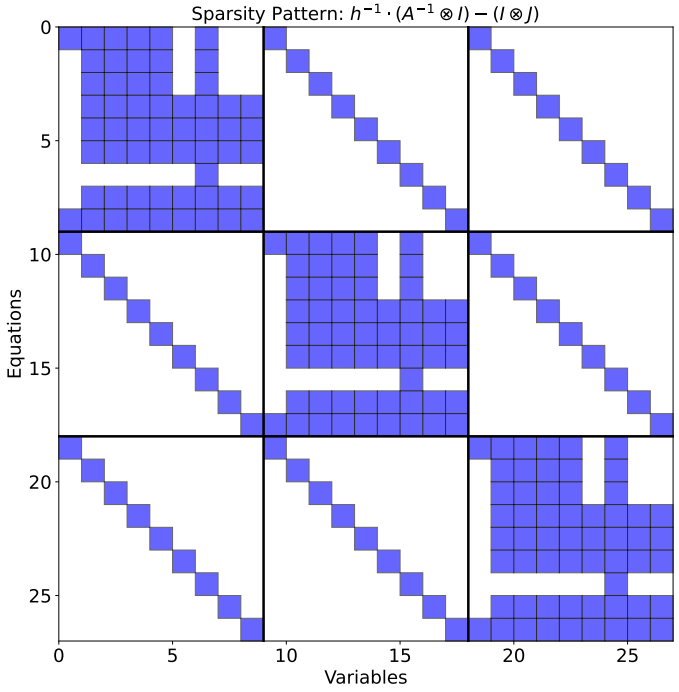
$$\boldsymbol{0} = \boldsymbol{Z} - h(A \otimes I_n)\boldsymbol{F}(\boldsymbol{Z})$$

Jacobian

$$\frac{\partial \boldsymbol{G}_Z}{\partial \boldsymbol{Z}} = I_s \otimes I_n - h\, A \otimes J$$

→ Reduces absorption effects by a bit

EFFICIENT NLS FOR FIRK: DIFFERENTIATION FORMULATION



Nonlinear System

$$\mathbf{0} = \boldsymbol{Z} - h(A \otimes I_n)\boldsymbol{F}(\boldsymbol{Z})$$
$$\iff \mathbf{0} = h^{-1}(A^{-1} \otimes I_n)\boldsymbol{Z} - \boldsymbol{F}(\boldsymbol{Z})$$

Jacobian

$$\frac{\partial \boldsymbol{G}_D}{\partial \boldsymbol{Z}} = h^{-1}A^{-1} \otimes I_n - I_s \otimes J$$

- Still a $3n \times 3n$ system
- Sparsity is way better already
- This formulation is used in Direct Collocation Dynamic Optimization

THE BLOCK-DIAGONAL TRANSFORMATION

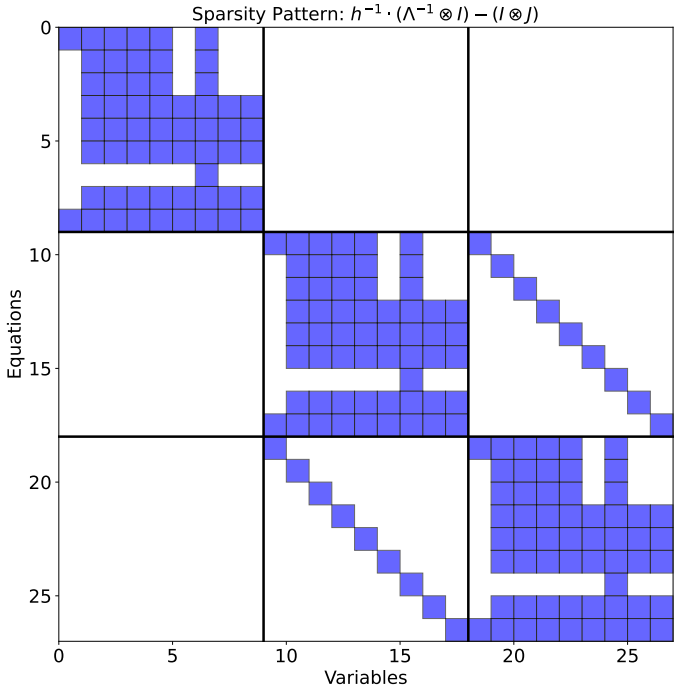
- Find a block-diagonal Transformation $A^{-1} = T\Lambda T^{-1}$
- Example: 3-step Radau IIA with $\gamma \approx 3.63783, \alpha \approx 2.68108, \beta \approx 3.05043$

$$A^{-1} = T\Lambda T^{-1} \text{ with } \Lambda = \begin{pmatrix} \gamma_1 & 0 & 0 \\ 0 & \alpha_1 & -\beta_1 \\ 0 & \beta_1 & \alpha_1 \end{pmatrix}, \; T = \begin{pmatrix} 0.094438 & -0.141255 & 0.030029 \\ 0.250213 & 0.204129 & -0.382942 \\ 1 & 1 & 0 \end{pmatrix}$$

- Set $\boldsymbol{W} := (T^{-1} \otimes I_n)\boldsymbol{Z}$ and it follows that

$$\begin{aligned} \mathbf{0} &= h^{-1} \left(A^{-1} \otimes I_n\right) \boldsymbol{Z} - \boldsymbol{F}(\boldsymbol{Z}) \\ &= h^{-1} \left(T\Lambda T^{-1} \otimes I_n\right) \boldsymbol{Z} - \boldsymbol{F}(\boldsymbol{Z}) \\ &= h^{-1} \left(T\Lambda \otimes I_n\right) \boldsymbol{W} - \boldsymbol{F}((T \otimes I_n)\boldsymbol{W}) \\ &= h^{-1} \left(\Lambda \otimes I_n\right) \boldsymbol{W} - (T^{-1} \otimes I_n)\boldsymbol{F}((T \otimes I_n)\boldsymbol{W}) \end{aligned}$$

EFFICIENT NLS FOR FIRK: W-SPACE FORMULATION



Nonlinear System

$$\mathbf{0} = h^{-1}(\Lambda \otimes I_n)\boldsymbol{W} - (T^{-1} \otimes I_n)\boldsymbol{F}((T \otimes I_n)\boldsymbol{W})$$

Jacobian

$$\frac{\partial \boldsymbol{G}_W}{\partial \boldsymbol{W}} = h^{-1}(\Lambda \otimes I_n) - (I_s \otimes J)$$

- System is split into one $n \times n$ and one $2n \times 2n$ system
- Runtime is reduced to $\mathcal{O}(n^3 + 8n^3) = \mathcal{O}(9n^3)$
- Overhead of matrix-vector products is just $\mathcal{O}(s^2 n)$

$\rightarrow$ 3 times faster than the naive implementation

EFFICIENT NLS FOR FIRK: COMPLEX ARITHMETIC

- Each complex conjugate eigenpair creates $2n \times 2n$ real systems

$$\begin{pmatrix} A & -B \\ B & A \end{pmatrix} \begin{pmatrix} \Delta \boldsymbol{w}_1 \\ \Delta \boldsymbol{w}_2 \end{pmatrix} = \begin{pmatrix} \boldsymbol{r}_1 \\ \boldsymbol{r}_2 \end{pmatrix}$$

- Solving the linear system is equivalent to solving the $n \times n$ complex system

$$(A + \mathrm{i}B)(\Delta \boldsymbol{w}_1 + \mathrm{i}\Delta \boldsymbol{w}_2) = \boldsymbol{r}_1 + \mathrm{i}\boldsymbol{r}_2$$

- Just $\mathcal{O}(n^3 + 4n^3) = \mathcal{O}(5n^3)$ flops for Radau IIA 3-step - more than 5 times faster!!

CONVERGENCE, DIVERGENCE AND JACOBIAN CALLBACKS

- New convergence condition for the Newton loop, which is closely tied to the integrators acceptance / rejection norm
- Main idea: if the estimated residual obeys a stronger condition than the states for acceptance, then the NLS is converged

→ Avoids solving the NLS to unnecessary precision - in some sense to the precision that is exactly required!

- Detect divergence of the Newton loop early
- Keep the Jacobian constant, if the convergence rate is sufficiently fast

→ Jacobians of linear ODEs are evaluated just once

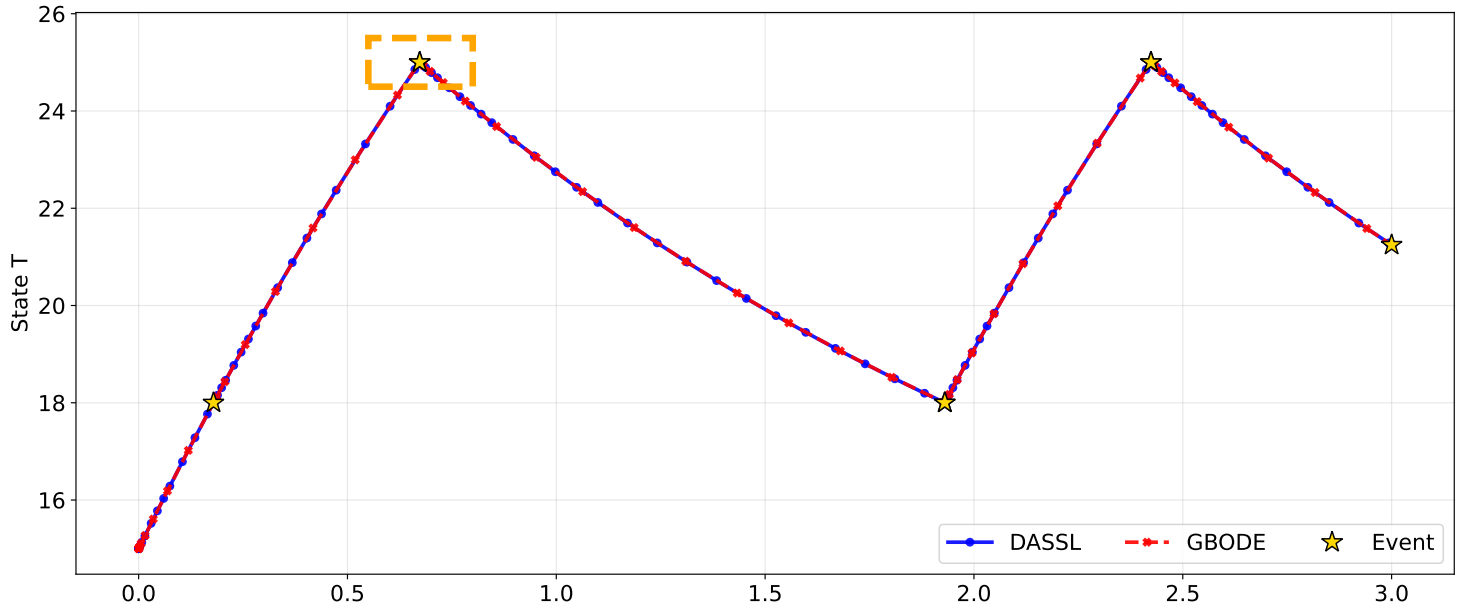
- Update start values for all collocation methods

A TAKE ON EVENTS

- After an event, BDF methods like DASSL or IDA have to redo bootstrapping and effectively fall back to an implicit Euler method

→ Step size must be completely reset to a tiny value

- This is often unnecessary and very expensive if you have a lot events



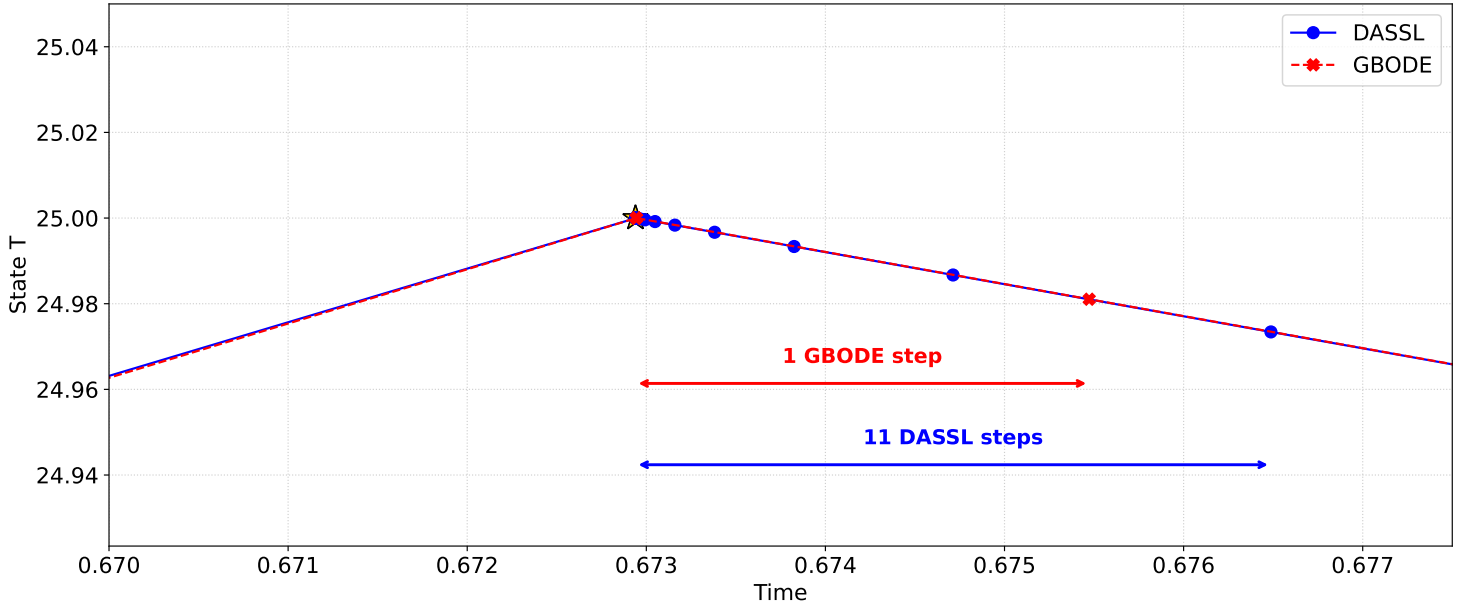
A TAKE ON EVENTS

- Runge-Kutta methods are 1-step methods and do not require bootstrapping

→ Step size must not be reset

→ Implemented a strategy that sets $h_{\text{new}} := \max\{0.1h_{\text{old}}, h_{\text{init}}\}$

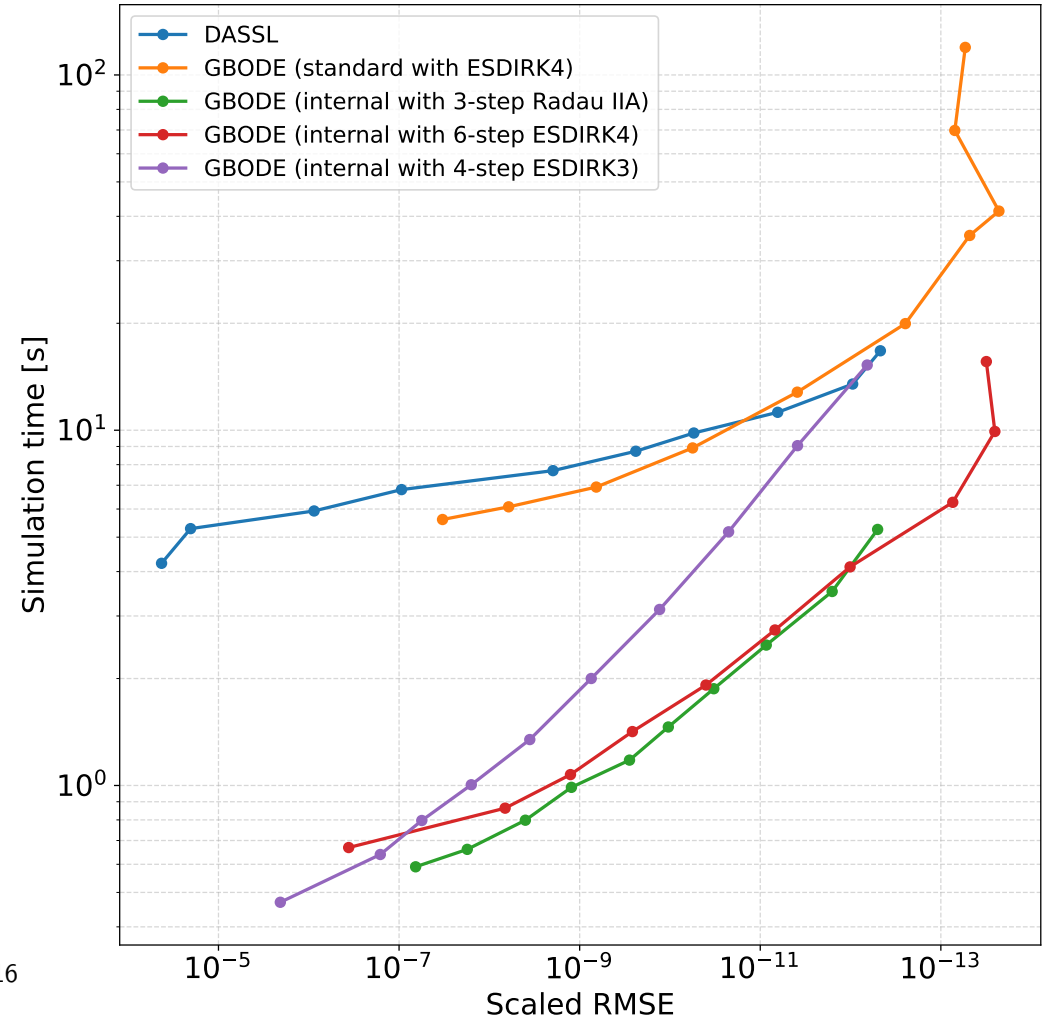
- Where to check zero-crossings?



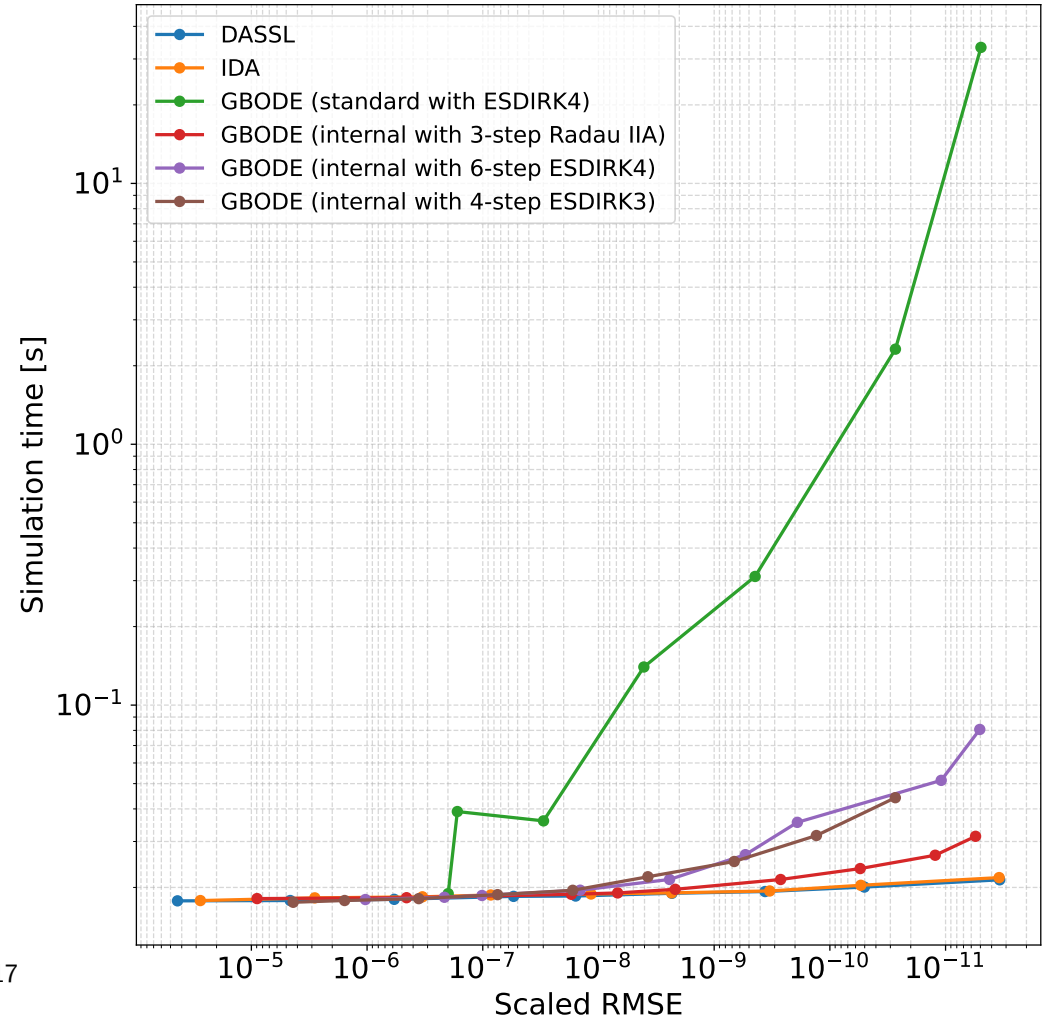
PERFORMANCE

- We test the new flag `-gbnls=internal` on several examples
- Always set `-gbnls=internal` and `-gberr=embedded`
- The tested methods are `-gbm=radauIIA3`, `-gbm=esdirk4` and `-gbm=esdirk3`
- IDA and DASSL are also included in the benchmark
- Tests are run on the latest OpenModelica master
- Timings are averaged over several runs and the error is given as the scaled RMSE with respect to the reference (IDA or DASSL) with tolerance 10^{-12}

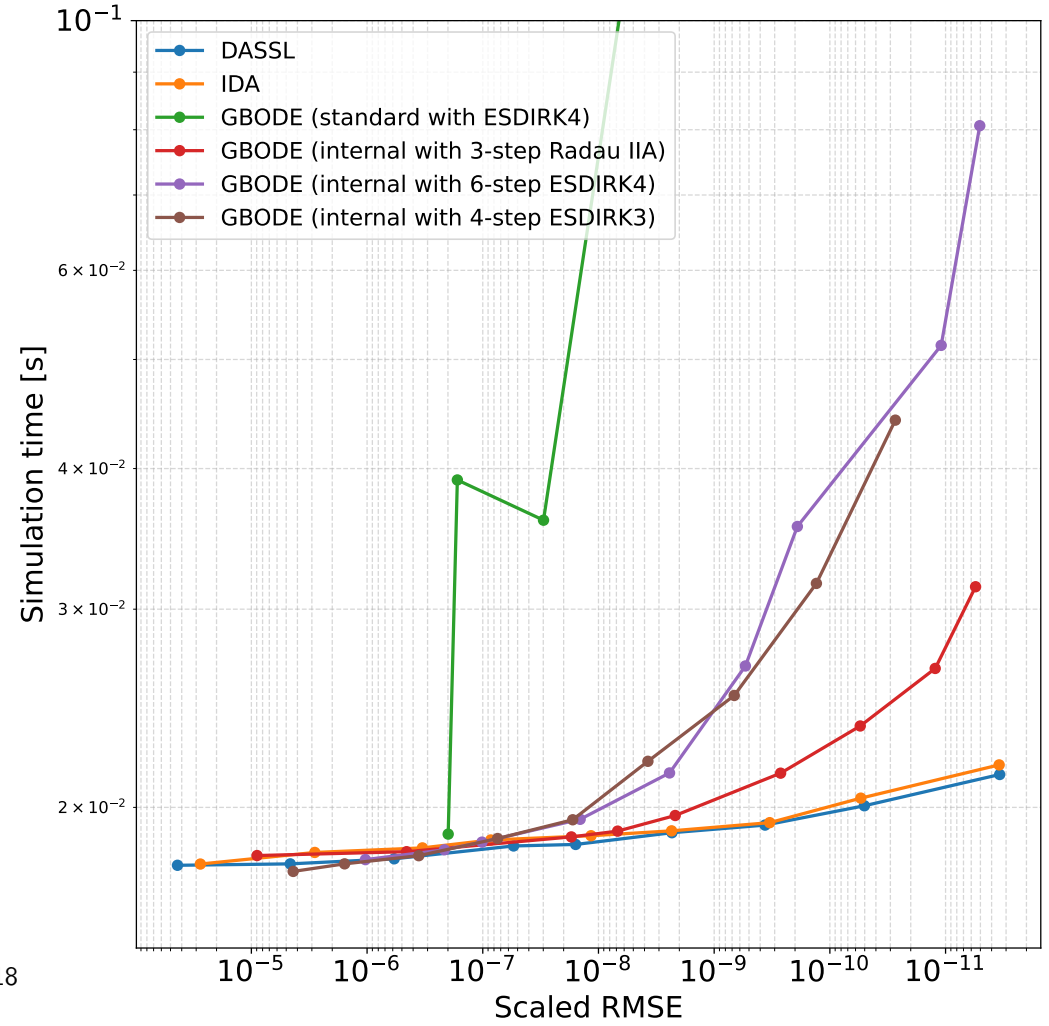
EXOGENOUS HEATING SYSTEM



ROBERTSON REACTION I



ROBERTSON REACTION II



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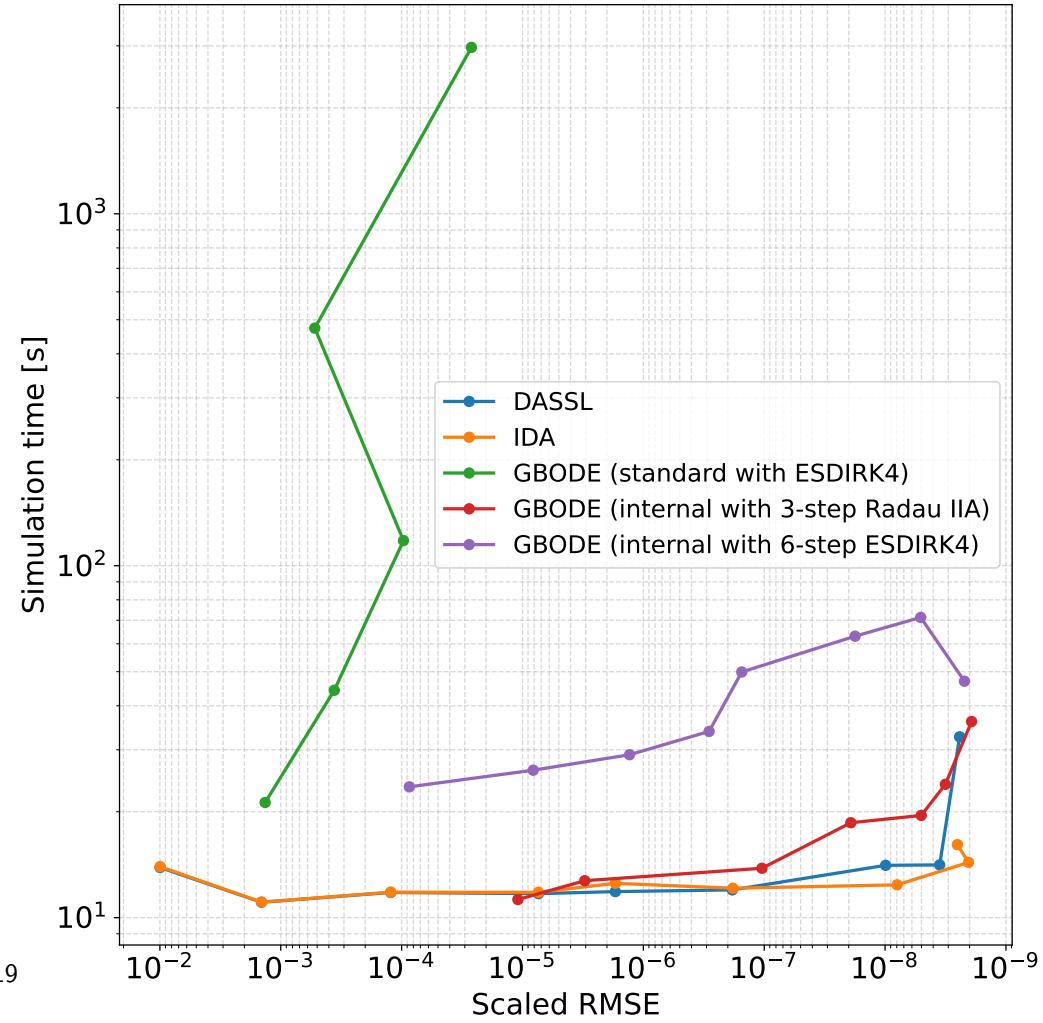

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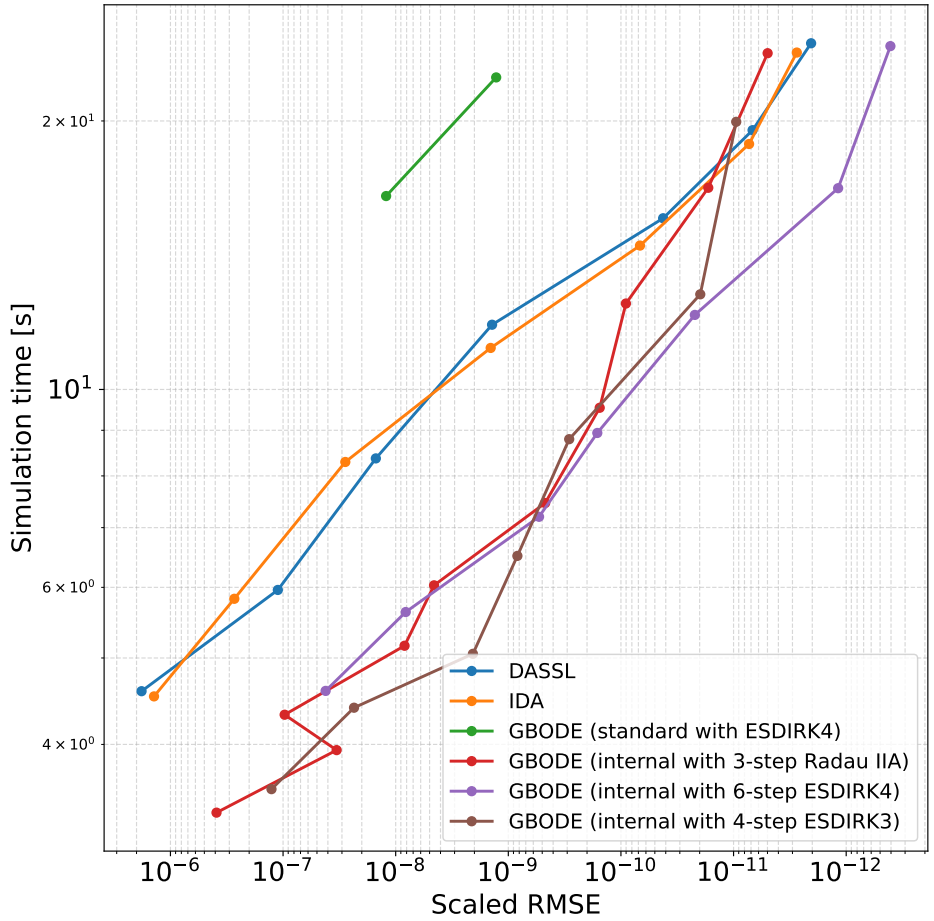

SUMMARY

- What does `-gbnls=internal` include?
  - Efficient NLS for FIRK methods
  - New convergence, divergence and Jacobian recomputation strategies
  - Experimental step-size selection after events

→ Its suggested to use the latest master or nightly and `-gberr=embedded` `-gbm=radauIIA3`, if you want to try it

- If using the latest release, you must use a symbolic Jacobian
- Still to do
  - Tuning of parameters
  - Stage-Value Predictors for (E)SDIRK methods
  - Better event handling in GBODE
  - Extend `-gbnls=internal` to multi-rate simulations