
SIRK → SERK → DIRK → SDIRK → SIRK

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Optimism and Pessimism

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c_1	a_{11}	0	0	\dots	0
c_2	a_{21}	a_{22}	0	\dots	0
c_3	a_{31}	a_{32}	a_{33}	\dots	0
\vdots	\vdots	\vdots	\vdots	\vdots	\vdots
c_s	a_{s1}	a_{s2}	a_{s3}	\dots	a_{ss}
	b_1	b_2	b_3	\dots	b_s

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For example the following method has order 5:

0				
$\frac{1}{4}$	$\frac{1}{8}$	$\frac{1}{8}$		
$\frac{7}{10}$	$\frac{1}{100}$	$\frac{14}{25}$	$\frac{3}{20}$	
1	$\frac{2}{7}$	0	$\frac{5}{7}$	
	$\frac{1}{14}$	$\frac{32}{81}$	$\frac{250}{567}$	$\frac{5}{54}$

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$$R(z) = \frac{N(z)}{(1 - \lambda z)^s}$$

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$$R(z) = \frac{N(z)}{(1 - \lambda z)^s}$$

Knowing which cases lead to A-stable methods is of crucial importance in the solution of stiff problems.

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λ	λ		
$\frac{1}{2}(1 + \lambda)$	$\frac{1}{2}(1 - \lambda)$	λ	
1	$\frac{1}{4}(-6\lambda^2 + 16\lambda - 1)$	$\frac{1}{4}(6\lambda^2 - 20\lambda + 5)$	λ
	$\frac{1}{4}(-6\lambda^2 + 16\lambda - 1)$	$\frac{1}{4}(6\lambda^2 - 20\lambda + 5)$	λ

where $\lambda \approx 0.4358665215$ satisfies $\frac{1}{6} - \frac{3}{2}\lambda + 3\lambda^2 - \lambda^3 = 0$.

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This work is part of a practical project to obtain efficient stiff solvers of moderate order.

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The answer lies in the inclusion of a transformation to Jordan canonical form into the computation.

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$$\bar{A} = \lambda(I - J) = \lambda \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 & 0 \\ -1 & 1 & 0 & \cdots & 0 & 0 \\ 0 & -1 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & 0 \\ 0 & 0 & 0 & \cdots & -1 & 1 \end{bmatrix}$$

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where e is the vector in \mathbb{R}^n with every component equal to 1 and Y has subvectors Y_i , $i = 1, 2, \dots, s$

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The following table summarises the costs

LU factorisation	$s^3 N^3$	
Backsolves	$s^2 N^2$	

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where the vector powers are interpreted component by component.

This is equivalent to

$$A^k c^0 = \frac{1}{k!} c^k, \quad k = 1, 2, \dots, s \quad (*)$$

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$$(A - \lambda I)^s c^0 = 0$$

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Substitute from (*) and it is found that

$$\sum_{i=0}^s \frac{1}{i!} \binom{s}{i} (-\lambda)^{s-i} c^i = 0.$$

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The question now is, how should λ be chosen?

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However, we first look at the transformation matrix T for efficient implementation.

Define the matrix T as follows:

$$T = \begin{bmatrix} L_0(\xi_1) & L_1(\xi_1) & L_2(\xi_1) & \cdots & L_{s-1}(\xi_1) \\ L_0(\xi_2) & L_1(\xi_2) & L_2(\xi_2) & \cdots & L_{s-1}(\xi_2) \\ L_0(\xi_3) & L_1(\xi_3) & L_2(\xi_3) & \cdots & L_{s-1}(\xi_3) \\ \vdots & \vdots & \vdots & & \vdots \\ L_0(\xi_s) & L_1(\xi_s) & L_2(\xi_s) & \cdots & L_{s-1}(\xi_s) \end{bmatrix}$$

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It can be shown that for a SIRK method

$$T^{-1}AT = \lambda(I - J)$$

Improving SIRK methods

There are two ways in which SIRK methods can be generalized

In the first of these we add extra diagonally implicit stages so that the coefficient matrix looks like this:

$$\begin{bmatrix} \hat{A} & 0 \\ W & \lambda I \end{bmatrix},$$

where the spectrum of the $p \times p$ submatrix \hat{A} is

$$\sigma(\hat{A}) = \{\lambda\}$$

For $s - p = 1, 2, 3, \dots$ we get improvements to the behaviour of the methods

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We will examine effective order in more detail.

Doubly companion matrices

Matrices like the following are “companion matrices” for the polynomial

$$z^n + \alpha_1 z^{n-1} + \dots + \alpha_n$$

$$\begin{bmatrix} -\alpha_1 & -\alpha_2 & -\alpha_3 & \dots & -\alpha_{n-1} & -\alpha_n \\ 1 & 0 & 0 & \dots & 0 & 0 \\ 0 & 1 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 0 & 0 \\ 0 & 0 & 0 & \dots & 1 & 0 \end{bmatrix}$$

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or
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$$z^n + \beta_1 z^{n-1} + \dots + \beta_n,$$

respectively:

$$\begin{bmatrix} -\alpha_1 & -\alpha_2 & -\alpha_3 & \dots & -\alpha_{n-1} & -\alpha_n \\ 1 & 0 & 0 & \dots & 0 & 0 \\ 0 & 1 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 0 & 0 \\ 0 & 0 & 0 & \dots & 1 & 0 \end{bmatrix}, \quad \begin{bmatrix} 0 & 0 & 0 & \dots & 0 & -\beta_n \\ 1 & 0 & 0 & \dots & 0 & -\beta_{n-1} \\ 0 & 1 & 0 & \dots & 0 & -\beta_{n-2} \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 0 & -\beta_2 \\ 0 & 0 & 0 & \dots & 1 & -\beta_1 \end{bmatrix}$$

Their characteristic polynomials can be found from $\det(I - zA) = \alpha(z)$ or $\beta(z)$, respectively, where,

$$\alpha(z) = 1 + \alpha_1 z + \dots + \alpha_n z^n, \quad \beta(z) = 1 + \beta_1 z + \dots + \beta_n z^n.$$

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A matrix with both α and β terms:

$$X = \begin{bmatrix} -\alpha_1 & -\alpha_2 & -\alpha_3 & \dots & -\alpha_{n-1} & -\alpha_n - \beta_n \\ 1 & 0 & 0 & \dots & 0 & -\beta_{n-1} \\ 0 & 1 & 0 & \dots & 0 & -\beta_{n-2} \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 0 & -\beta_2 \\ 0 & 0 & 0 & \dots & 1 & -\beta_1 \end{bmatrix},$$

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is known as a “doubly companion matrix” and has characteristic polynomial defined by

$$\det(I - zX) = \alpha(z)\beta(z) + O(z^{n+1})$$

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$$\Psi^{-1} = \begin{bmatrix} 1 & \lambda + \alpha_1 & \lambda^2 + \alpha_1\lambda + \alpha_2 & \cdots \\ 0 & 1 & 2\lambda + \alpha_1 & \cdots \\ 0 & 0 & 1 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

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We have a similar expression for Ψ :

$$\Psi = \begin{bmatrix} \ddots & \vdots & \vdots & \vdots \\ \dots & 1 & 2\lambda + \beta_1 & \lambda^2 + \beta_1\lambda + \beta_2 \\ \dots & 0 & 1 & \lambda + \beta_1 \\ \dots & 0 & 0 & 1 \end{bmatrix}$$

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The Jordan form is $\Psi^{-1}X\Psi = J + \lambda I$, where $J_{ij} = \delta_{i,j+1}$.

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We will illustrate this operation in a table

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We will illustrate this operation in a table, where we also introduce the special member $E \in G$.

i t_i

1



2



3



4



5



6



7



8



$r(t_i)$	i	t_i
1	1	•
2	2	• •
3	3	• • •
3	4	• • • •
4	5	• • • • •
4	6	• • • • • •
4	7	• • • • • • •
4	8	• • • • • • • •

$r(t_i)$	i	t_i	$\alpha(t_i)$	$\beta(t_i)$
1	1	•	α_1	β_1
2	2	⋮	α_2	β_2
3	3	∨	α_3	β_3
3	4	⋮	α_4	β_4
4	5	∨	α_5	β_5
4	6	∨	α_6	β_6
4	7	∨	α_7	β_7
4	8	⋮	α_8	β_8

$r(t_i)$	i	t_i	$\alpha(t_i)$	$\beta(t_i)$	$(\alpha\beta)(t_i)$
1	1	•	α_1	β_1	$\alpha_1 + \beta_1$
2	2	• •	α_2	β_2	$\alpha_2 + \alpha_1\beta_1 + \beta_2$
3	3	• • •	α_3	β_3	$\alpha_3 + \alpha_1^2\beta_1 + 2\alpha_1\beta_2 + \beta_3$
3	4	• • • •	α_4	β_4	$\alpha_4 + \alpha_2\beta_1 + \alpha_1\beta_2 + \beta_4$
4	5	• • • • •	α_5	β_5	$\alpha_5 + \alpha_1^3\beta_1 + 3\alpha_1^2\beta_2 + 3\alpha_1\beta_3 + \beta_5$
4	6	• • • • •	α_6	β_6	$\alpha_6 + \alpha_1\alpha_2\beta_1 + (\alpha_1^2 + \alpha_2)\beta_2 + \alpha_1(\beta_3 + \beta_4) + \beta_6$
4	7	• • • • • •	α_7	β_7	$\alpha_7 + \alpha_3\beta_1 + \alpha_1^2\beta_2 + 2\alpha_1\beta_4 + \beta_7$
4	8	• • • • • • •	α_8	β_8	$\alpha_8 + \alpha_4\beta_1 + \alpha_2\beta_2 + \alpha_1\beta_4 + \beta_8$

$r(t_i)$	i	t_i	$\alpha(t_i)$	$\beta(t_i)$	$(\alpha\beta)(t_i)$	$E(t_i)$
1	1	•	α_1	β_1	$\alpha_1 + \beta_1$	1
2	2	• •	α_2	β_2	$\alpha_2 + \alpha_1\beta_1 + \beta_2$	$\frac{1}{2}$
3	3	• • •	α_3	β_3	$\alpha_3 + \alpha_1^2\beta_1 + 2\alpha_1\beta_2 + \beta_3$	$\frac{1}{3}$
3	4	• • • •	α_4	β_4	$\alpha_4 + \alpha_2\beta_1 + \alpha_1\beta_2 + \beta_4$	$\frac{1}{6}$
4	5	• • • • •	α_5	β_5	$\alpha_5 + \alpha_1^3\beta_1 + 3\alpha_1^2\beta_2 + 3\alpha_1\beta_3 + \beta_5$	$\frac{1}{4}$
4	6	• • • • •	α_6	β_6	$\alpha_6 + \alpha_1\alpha_2\beta_1 + (\alpha_1^2 + \alpha_2)\beta_2 + \alpha_1(\beta_3 + \beta_4) + \beta_6$	$\frac{1}{8}$
4	7	• • • • • •	α_7	β_7	$\alpha_7 + \alpha_3\beta_1 + \alpha_1^2\beta_2 + 2\alpha_1\beta_4 + \beta_7$	$\frac{1}{12}$
4	8	• • • • • • •	α_8	β_8	$\alpha_8 + \alpha_4\beta_1 + \alpha_2\beta_2 + \alpha_1\beta_4 + \beta_8$	$\frac{1}{24}$

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If α is defined from the elementary weights for a Runge-Kutta method then order p can be written as

$$\alpha G_p = EG_p.$$

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If α is defined from the elementary weights for a Runge-Kutta method then order p can be written as

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Effective order p is defined by the existence of β such that

$$\beta \alpha G_p = E \beta G_p.$$

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Thus, the benefits of high order can be enjoyed by high effective order.

We analyse the conditions for effective order 4.

Without loss of generality assume $\beta(t_1) = 0$.

i	$(\beta\alpha)(t_i)$	$(E\beta)(t_i)$
1	α_1	1
2	$\beta_2 + \alpha_2$	$\frac{1}{2} + \beta_2$
3	$\beta_3 + \alpha_3$	$\frac{1}{3} + 2\beta_2 + \beta_3$
4	$\beta_4 + \beta_2\alpha_1 + \alpha_4$	$\frac{1}{6} + \beta_2 + \beta_4$
5	$\beta_5 + \alpha_5$	$\frac{1}{4} + 3\beta_2 + 3\beta_3 + \beta_5$
6	$\beta_6 + \beta_2\alpha_2 + \alpha_6$	$\frac{1}{8} + \frac{3}{2}\beta_2 + \beta_3 + \beta_4 + \beta_6$
7	$\beta_7 + \beta_3\alpha_1 + \alpha_7$	$\frac{1}{12} + \beta_2 + 2\beta_4 + \beta_7$
8	$\beta_8 + \beta_4\alpha_1 + \beta_2\alpha_2 + \alpha_8$	$\frac{1}{24} + \frac{1}{2}\beta_2 + \beta_4 + \beta_8$

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Once α is known, there remain 3 conditions on β .

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The 5 order conditions, written in terms of the Runge-Kutta tableau, are

$$\sum b_i = 1$$

$$\sum b_i c_i = \frac{1}{2}$$

$$\sum b_i a_{ij} c_j = \frac{1}{6}$$

$$\sum b_i a_{ij} a_{jk} c_k = \frac{1}{24}$$

$$\sum b_i c_i^2 (1 - c_i) + \sum b_i a_{ij} c_j (2c_i - c_j) = \frac{1}{4}$$

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To construct a SIRK method with effective order s , and with a specific choice of the abscissa vector c and a specific value of λ , use the properties of doubly companion matrices.

Construction of methods

- Choose λ and abscissa vector c .

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- Define $\beta_1, \beta_2, \dots, \beta_s$ so that the zeros of the polynomial

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- Define $\alpha_1, \alpha_2, \dots, \alpha_s$ so that
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- Construct the corresponding doubly companion matrix X

-
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$$C = \begin{bmatrix} 1 & c_1 & \frac{1}{2!}c_1^2 & \cdots & \frac{1}{(s-1)!}c_1^{s-1} \\ 1 & c_2 & \frac{1}{2!}c_2^2 & \cdots & \frac{1}{(s-1)!}c_2^{s-1} \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & c_s & \frac{1}{2!}c_s^2 & \cdots & \frac{1}{(s-1)!}c_s^{s-1} \end{bmatrix}$$

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$$\widehat{b}^T = \left[\frac{1}{1!}, \frac{\alpha_1}{1!} + \frac{1}{2!}, \frac{\alpha_2}{1!} + \frac{\alpha_1}{2!} + \frac{1}{3!}, \cdots, \frac{\alpha_{s-1}}{1!} + \cdots + \frac{1}{s!} \right]$$

Final comments

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- Lastly: I will report on my efforts to document links between the two of us

Proof that my Nørsett number is 2

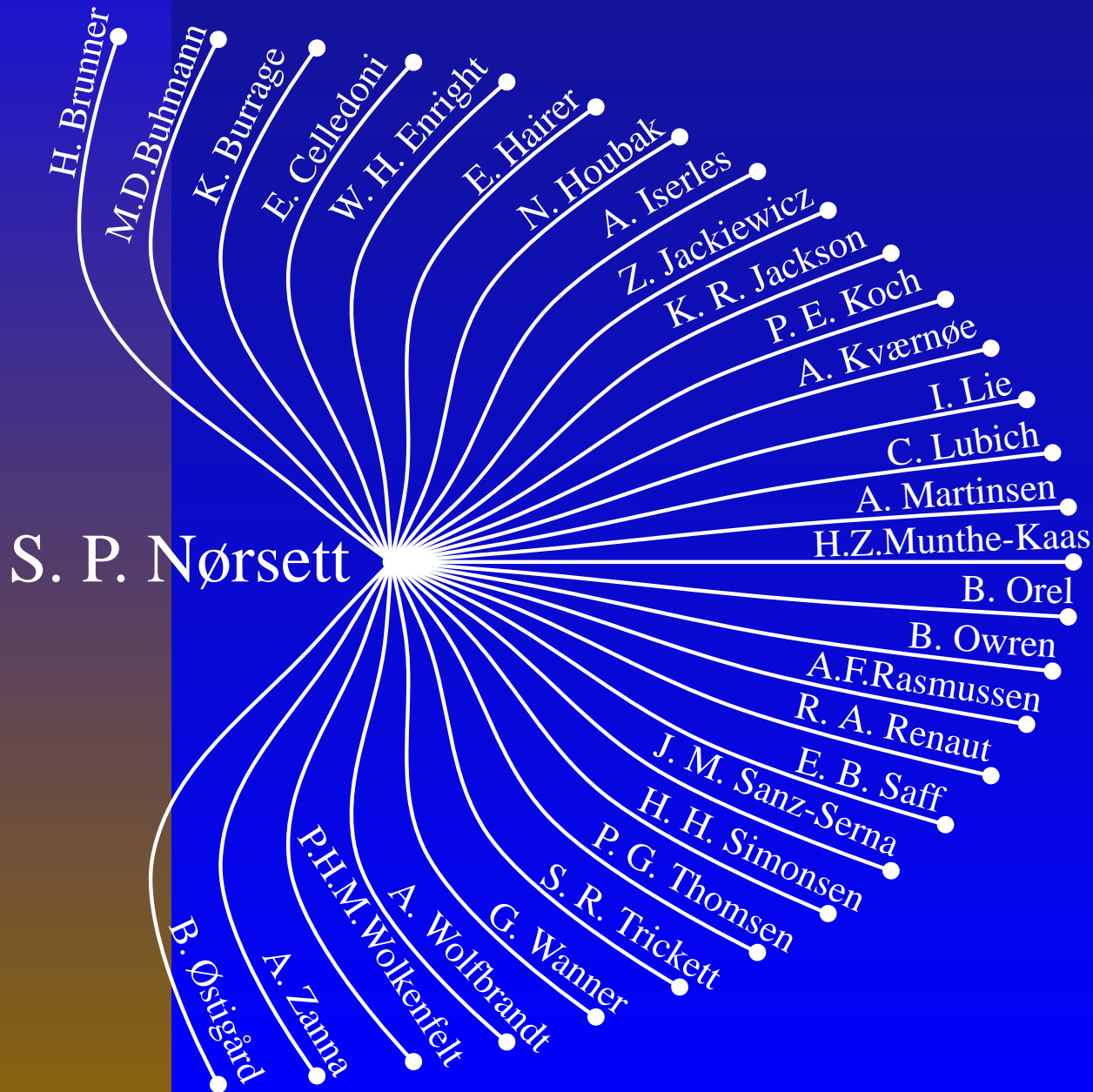
S. P. Nørsett •

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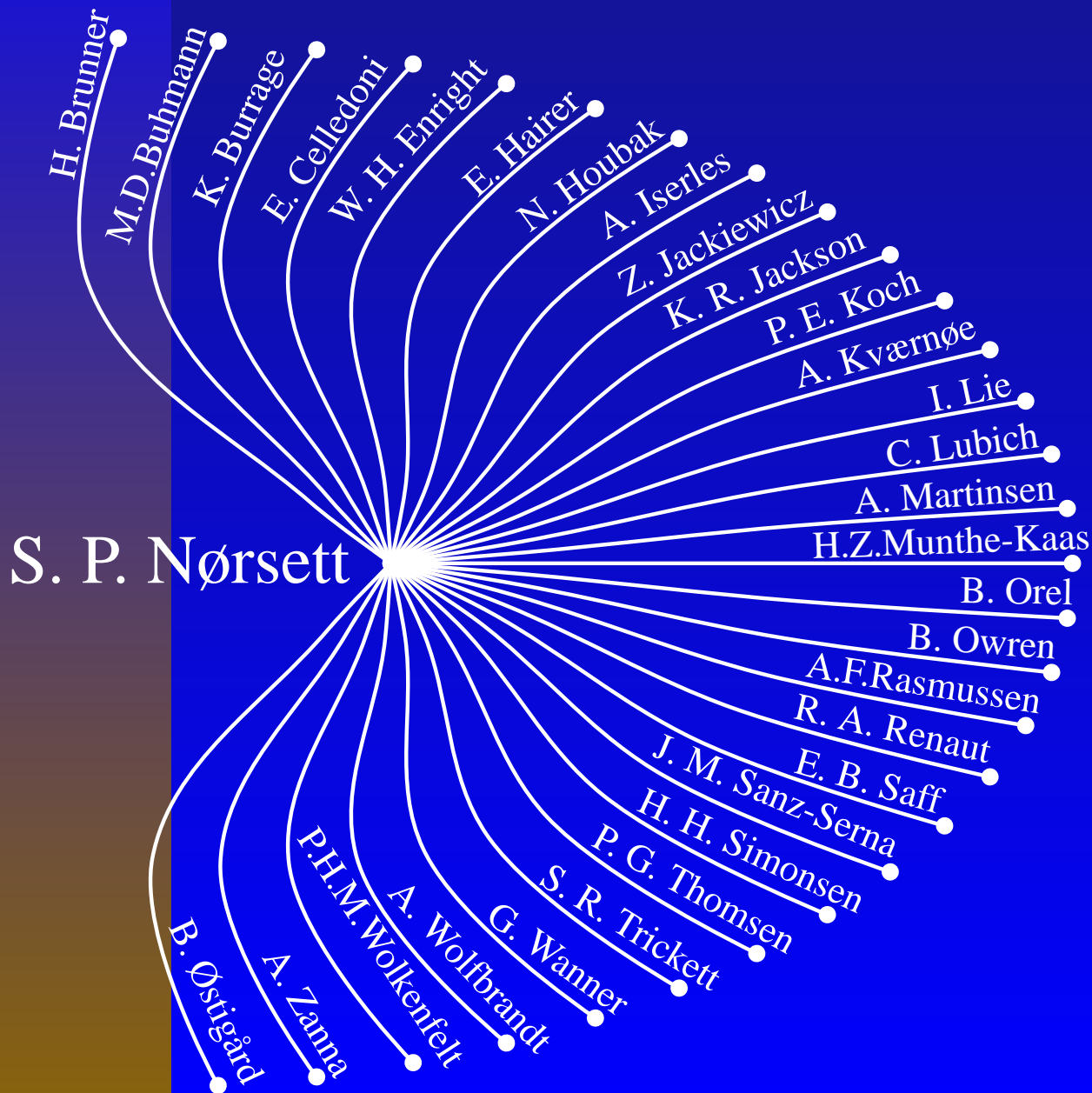
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J. C. B. •

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