LECTURE 10 (24/02/25)

IN THE LAST PART OF THE LECTURE WE SAW THAT AN ADR ON A RECTANGLE DOMAIN WITH SUITABLE BDY CONDITIONS CAN BE DISCRETIZED IN SPACE AS

$$\begin{cases} u'(t) = K u(t) + g(u(t)) \\ u(0) = u_0 \end{cases}$$

LARGE AND SPARSE MATRIX

WHERE

$$K = I^y \otimes (\underbrace{\delta D_2^x + \alpha D_1^x}_{A}) + (\underbrace{\delta D_2^y + \alpha D_1^y}_{B}) \otimes I^x$$

$I^x = I^y = I$

THE QUESTION IS

CAN WE EXPLOIT THE STRUCTURE OF K TO ACCELLERATE OUR EXPONENTIAL INTEGRATORS?

EXPLOITING THE STRUTURE OF K IN LAWSON METHODS

WE RECALL THE LAWSON EULER METHOD:

$$u_{n+1} = e^{\tau K}(u_n + \tau g(u_n)) \qquad (LE)$$

WE COULD USE ANY METHOD FOR COMPUTING THE ACTION OF THE MATRIX EXPONENTIAL (EXPMV, KIOPS, ...), BUT WE DO MORE.

IN PARTICULAR WE CAN PROVE THAT

$$e^{\tau K} = e^{\tau(I \otimes A + B \otimes I)} = e^{\tau B} \otimes e^{\tau A}$$

$(C \otimes D)(E \otimes F) = (CE) \otimes (DF)$

TO SEE THIS, WE NOTICE THAT $I \otimes A$ AND $B \otimes I$ COMMUTE (THANKS TO THE SO-CALLED MIXED PRODUCT PROPERTY OF $\otimes$)

$$(I \otimes A)(B \otimes I) = B \otimes A \qquad (B \otimes I)(I \otimes A) = B \otimes A$$

THEREFORE I CAN SPLIT THE EXPONENTIAL AS

SCALARS CAN BE PUT INSIDE $\otimes$

$$e^{\tau K} = e^{\tau(I\otimes A + B\otimes I)} = e^{\tau(I\otimes A)} e^{\tau(B\otimes I)} = e^{I\otimes(\tau A)} e^{(\tau B)\otimes I}$$

NOW WE OBSERVE THAT

$$e^{I\otimes X} = I\otimes e^{X} \quad (*) \qquad\qquad e^{X\otimes I} = e^{X}\otimes I$$

HINT $\Rightarrow$ TAYLOR EXPANSION + MIXED PRODUCT PROPERTY

$$e^{I\otimes X} = \sum_{i=0}^{+\infty} \frac{(I\otimes X)^i}{i!} = \sum_{i=0}^{+\infty} I\otimes \frac{X^i}{i!} = I\otimes \sum_{i=0}^{+\infty}\frac{X^i}{i!} = I\otimes e^{X}$$

THEN, BY USING $(*)$ WE GET

MIXED PRODUCT

$$e^{I\otimes(\tau A)} e^{(\tau B)\otimes I} = \left(I\otimes e^{\tau A}\right)\left(e^{\tau B}\otimes I\right) = e^{\tau B}\otimes e^{\tau A}$$

WHICH IS WHAT WE WANTED.

IN OUR EXPONENTIAL INTEGRATOR WE WOULD HAVE TO COMPUTE

$$e^{\tau K} v = \left(e^{\tau B}\otimes e^{\tau A}\right) v$$

FULL AND COMPUTING $\otimes$ IS COMPUTATIONALLY TOO EXPENSIVE

FINALLY WE EMPLOY THE FOLLOWING KEY PROPERTY

$$(M_1\otimes M_2)d = \mathrm{vec}(M_2 D M_1^{T})$$

IF WORKING IN COMPLEX ARITHMETIC, THIS IS STILL TRANSPOSE, NOT CONJUGATE TRANSPOSE

WHERE M_1, M_2 ARE MATRICES, d IS A VECTOR SUCH THAT $\mathrm{vec}(D) = d$ (BEING D A MATRIX) AND vec IS THE OPERATOR WHICH STACKS BY COLUMNS THE INPUT MATRIX.

IN MATLAB $\mathrm{vec}(D) = D(:)$

THANKS TO THIS WE GET :

$$u_{n+1} = e^{\tau K}\left(u_n + \tau g(u_n)\right)$$

$$\Leftrightarrow$$

UP TO A VEC OPERATION

$$u_{n+1} = \left(e^{\tau B} \otimes e^{\tau A}\right)\left(u_n + \tau g(u_n)\right)$$

$$\Leftrightarrow$$

$$\boxed{U_{n+1} = e^{\tau A}\left(U_n + \tau G(U_n)\right) e^{\tau B^T}}$$

$u_{n+1} = \mathrm{vec}(U_{n+1})$

$\vdots$

WHICH IS THE MATRIX FORMULATION OF LAWSON EULER

ADVANTAGES

- WE DON'T HAVE TO BUILD THE LARGE-SIZED MATRIX K
- IT REQUIRES THE COMPUTATION OF SMALL SIZED MATRIX EXPONENTIALS (PADÉ / EXPM) AND BLAS3 PRODUCTS
- THIS FORMULATION GENERALIZES TO nD THANKS TO TENSOR MATRIX PRODUCTS (μ-MODE APPROACH)

DISADVANTAGES

- K MUST HAVE A KRONECKER PRODUCT STRUCTURE
- THIS IDEA DOES NOT GENERALIZE STRAIGHTFORWARDLY TO φ FUNCTIONS

THIS CAN BE SEEN AS A "SMART" WAY TO COMPUTE THE ACTION OF THE MATRIX EXPONENTIAL IN KRONECKER FORM

$$e^{K} v = \mathrm{vec}\left(e^{A} V e^{B}\right)$$

EXPLOITING KRONECKER PRODUCT FOR φ_1

UNFORTUNATELY, EVEN FOR COMMUTING MATRICES, WE ARE NOT ALLOWED TO SPLIT THE φ_1 FUNCTION (NOT EVEN TRUE IN THE SCALAR CASE)

$$e^{a+b} = e^{a} e^{b} \rightsquigarrow \varphi_1(a+b) \neq \varphi_1(a)\varphi_1(b)$$

$$\varphi_1(\tau K) = \varphi_1(\tau(I \otimes A + B \otimes I)) \neq \varphi_1(\tau(I \otimes A))\,\varphi_1(\tau(B \otimes I))$$

$$\overset{!}{=} \varphi_1(\tau B) \otimes \varphi_1(\tau A)$$

φ_1 IS AN ANALYTIC FUNCTION (TAYLOR EXPANSION + MIXED PRODUCT)

WE SAW THAT WE CAN REDUCE THE COMPUTATION OF THE ACTION OF THE φ_1 FUNCTION TO AN AUGMENTED MATRIX EXPONENTIAL

$$\tau\varphi_1(\tau K)v = \exp\left(\tau\begin{bmatrix}K & v\\ 0 & 0\end{bmatrix}\right)\begin{bmatrix}0\\ \vdots\\ 0\\ 1\end{bmatrix} = \exp(\tau\tilde{K})\begin{bmatrix}0\\ \vdots\\ 0\\ 1\end{bmatrix}$$

FIRST N ROWS

BUT $\tilde{K}$ IS NOT ANYMORE A KRONECKER SUM, SO WE CAN'T USE THE TECHNIQUE DESCRIBED BEFORE.

HOWEVER, WE COULD EXPLOIT THE RECURSIVE DEFINITION OF THE φ_1 FUNCTION

$$X\varphi_1(X) = e^X - I$$

IN OUR CASE

$$\tau K\varphi_1(\tau K) = e^{\tau K} - I$$

AND APPLYING A VECTOR v WE GET

$$\tau K\varphi_1(\tau K)v = e^{\tau K}v - v$$

$$\Longleftrightarrow$$

$$\tau(I\otimes A + B\otimes I)\underbrace{\varphi_1(\tau K)v}_{w \text{ (THE UNKNOWN)}} = e^{\tau(I\otimes A + B\otimes I)}v - v$$

$$\Longleftrightarrow$$

$$(I\otimes(\tau A))w + ((\tau B)\otimes I)w = \left(e^{\tau B}\otimes e^{\tau A}\right)v - v$$

BY MEANS OF OUR KEY PROPERTY WE GET

$$\Longleftrightarrow$$

$$(\tau A)W + W(\tau B)^T = e^{\tau A}Ve^{\tau B^T} - V$$

WHERE $w = \mathrm{vec}(W)$ AND $v = \mathrm{vec}(V)$

THE OBTAINED FORM IS A SYLVESTER (MATRIX) EQUATION FOR THE UNKNOWN W

$$M_1 X + X M_2 = M_3$$

THIS IS SOLVABLE IFF M_1 AND $-M_2$ HAVE DISJOINT SPECTRA

THANKS TO THIS WE CAN COMPUTE THE ACTION OF THE φ_1 FUNCTION (=> EXPONENTIAL EULER) AT THE COST OF A SYLVESTER SOLVE (+ SMALL MATRIX EXPONENTIALS). UNFORTUNATELY, THIS DOES NOT GENERALIZE EASILY TO nD. ON THE OTHER HAND, AT A COST OF SOLVING REPEATEDLY SYLVESTER EQUATION WE GENERALIZE TO $\varphi_2, \varphi_3, \ldots$.

ANOTHER APPROACH TO COMPUTE $\varphi_1(\tau K)\,v$ IS EXPLOITING THE INTEGRAL DEFINITION OF THE φ_1 FUNCTION

$$\varphi_1(\tau K)\,v = \int_0^1 e^{(1-\theta)\tau K}\, v \, d\theta$$

IF WE APPROXIMATE THE INTEGRAL WITH A SUITABLE QUADRATURE RULE (E.G., GAUSS) WE GET

$$\varphi_1(\tau K)\,v \simeq \sum_{i=1}^{m_q} e^{(1-\xi_i)\tau K}\, v\, w_i$$

QUADRATURE WEIGHTS

QUADRATURE NODES

ACTION OF THE MATRIX EXPONENTIAL IN KRONECKER FORM

WE CAN GENERALIZE THIS TO $\varphi_2, \varphi_3, \ldots$ (ACTIONS OF LINEAR COMBINATIONS) AND IT GENERALIZES TO nD.

DIRECTIONAL SPLITTING APPROACH

SINCE WE ARE IN THE CONTEXT OF EXPONENTIAL INTEGRATORS, WE ARE DOING A TIME MARCHING WE END UP WITH AN APPROXIMATED SOLUTION AT A CERTAIN ORDER OF CONVERGENCE ($\mathcal{O}(\tau^p)$)

TIME STEP SIZE

THEN, IN PRINCIPLE THERE IS NO NEED TO HAVE MATRIX FUNCTIONS AT MACHINE PRECISION (IT IS ENOUGH TO HAVE THEM BELOW THE PRECISION OF OUR INTEGRATOR).

COMING BACK TO THE φ_1 WE HAVE

$$\varphi_1(\tau K) \neq \varphi_1(I \otimes (\tau A))\, \varphi_1((\tau B) \otimes I)$$

YOU CAN SEE IT BY TAYLOR EXPANSION

DIRECTIONAL SPLITTING ERROR

BUT

$$\varphi_1(\tau K) = \varphi_1(I \otimes (\tau A))\, \varphi_1((\tau B) \otimes I) + \mathcal{O}(\tau^2)$$

$$= (I \otimes \varphi_1(\tau A))\,(\varphi_1(\tau B) \otimes I) + \mathcal{O}(\tau^2)$$

$$= \varphi_1(\tau B) \otimes \varphi_1(\tau A) + \mathcal{O}(\tau^2)$$

EQUAL

$$\varphi_1(\tau K)\, v \overset{\Longleftrightarrow}{=} \mathrm{vec}\left(\varphi_1(\tau A)\, V\, \varphi_1(\tau B^T)\right) + \mathcal{O}(\tau^2)$$

SINCE THE ERROR IS PROPORTIONAL TO τ^2, WE CAN "SAFELY" EMPLOY THIS APROXIMATION IN EXPONENTIAL INTEGRATORS UP TO SECOND ORDER.

IN TERMS OF CONVERGENCE ORDER (TRUE AT ODE LEVEL)

THE EXPONENTIAL EULER METHOD MAY BE "APPROXIMATED" AS

$$U_{n+1} = e^{\tau A} U_n e^{\tau B^T} + \tau \varphi_1(\tau A)\, G(U_n)\, \varphi_1(\tau B^T)$$

OR (NOT EQUIVALENTLY) AS

$$\overline{U}_{n+1} = \overline{U}_n + \tau \varphi_1(\tau A)\, F(\overline{U}_n)\, \varphi_1(\tau B^T).$$

THIS APPROACH MAY BE GENERALIZED TO HIGHER ORDER φ FUNCTIONS ($\varphi_2, \varphi_3, \dots$), TO nD, TO HIGHER ORDER INTEGRATORS.