11th International Computational Accelerator Physics Conference – ICAP 2012

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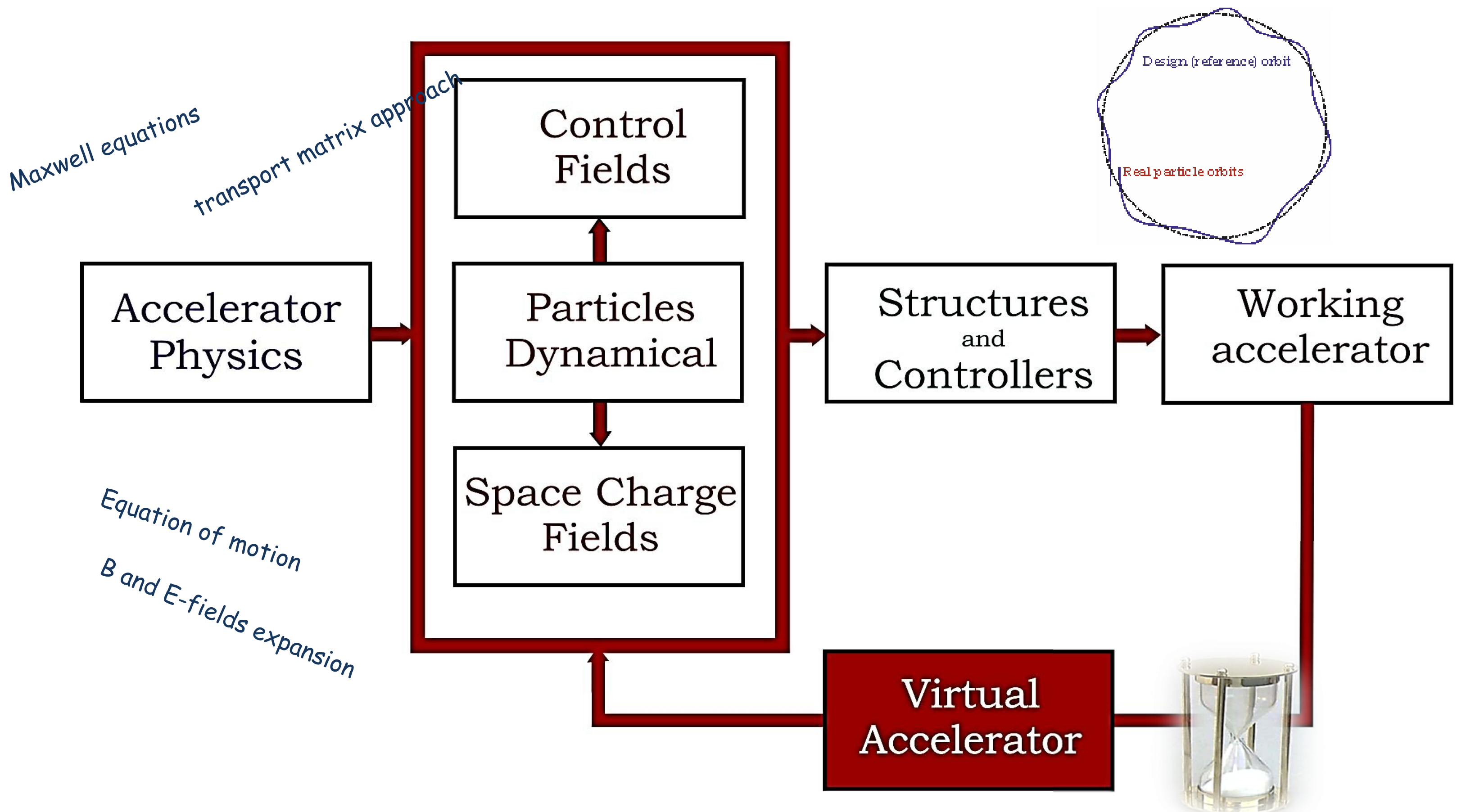
The Convergence and Accuracy of the Matrix Formalism Approximation

Structure of accelerator facilities modeling and control



From a physical model to a mathematical models

It is well known that the computational problems in beam physics can be divided into the following groups.

The first group of problem related to determining the required degree of approximation corresponding to the problem under study.

Second is based on calculation of the corresponding evolution operators in the framework of an used formalism.

The third class of problems connected with some specific tasks, for example such problems as the long beam evolution problem, the influence space charge, different aberrations correction and so on.

It is necessary to mention also problems embedding the selected numerical methods in some computational framework to carry out the necessary computational experiments, carry out optimization process and so on. We mean the well-known concept of a **virtual accelerator** have been used in the present time by various researchers.

From a physical model to a mathematical models

Let list the basic requirements for the methods that can be used to model the beam dynamics and the corresponding related problems.

First, the accuracy of approximation of the ideal mapping generated by the dynamical system. Here we should mention the problem: how estimate the closeness of ideal solutions and the corresponding approximate solutions?

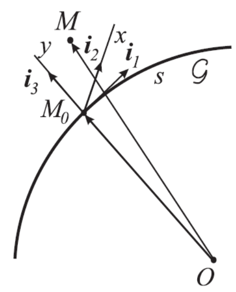
The second important demand is connected with the need to preserve the qualitative properties inherent in the dynamical system under study. For example, such as the symplectic property for Hamiltonian systems, conservation of exact and approximate integrals of motion and so on.

Finally, **the possibility of constructing accurate maps** for some practical classes of dynamical systems.

In particular, it is necessary to mention **one more problem** - the problem of **parallel and distributed computing** processes as in the map construction, and the dynamics of the beam as an ensemble.

From a physical model to a mathematical models

$$\mathbf{v} = \frac{d\mathbf{R}}{dt}, \qquad \frac{d\,(m\mathbf{v})}{dt} = q\left(\mathbf{E} + [\mathbf{v}\times\mathbf{B}]\right),$$



$$B_x = \frac{\partial\psi}{\partial x},\ B_y = \frac{\partial\psi}{\partial y},\ B_s = \frac{1}{1+hx}\frac{\partial\psi}{\partial s},$$

$$\psi(x,y,s) = \sum_{k,i=0}^{\infty} a_{ik}(s)\frac{x^i}{i!}\frac{y^k}{k!}.$$

$$\begin{aligned} a''_{ik} + kha''_{i,k-1} - kh'a'_{i,k-1} + a_{i+2,k} + a_{i,k+2} + \\ + (3k+1)ha_{i,k+1} + k(3k-1)h^2 a_{ik} + k(k-1)^2 h^3 a_{i,k-1} + \\ + 3kha_{i+2,k-1} + 3k(k-1)h^2 a_{i+2,k-2} + k(k-1)(k-2)h^3 a_{i+2,k-3} = 0. \end{aligned}$$

$$\begin{aligned} x'' - h^2 x = -h - \frac{x'(2hx' + h'x)}{1-hx} - \frac{1}{c\beta\gamma(1-hx)}\left((1-hx)^2 + x'^2 + y'^2\right)^{1/2} \times \\ \times \left(x'y'B_x - \left((1-hx)^2 + x'^2\right)B_y + (1-hx)y'B_s\right), \end{aligned}$$

$$\begin{aligned} y'' = -\frac{y'(2hx' + h'x)}{1-hx} + \frac{1}{c\beta\gamma(1-hx)}\left((1-hx)^2 + x'^2 + y'^2\right)^{1/2} \times \\ \times \left(-x'y'B_y - \left((1-hx)^2 + y'^2\right)B_x - (1-hx)x'B_s\right). \end{aligned}$$

$$\frac{d\mathbf{X}}{dt} = \mathbf{F}(\mathbf{X},t) = \mathbf{F}^{\mathrm{ext}}(\mathbf{B}^{\mathrm{ext}}(\mathbf{X},t), \mathbf{E}^{\mathrm{ext}}(\mathbf{X},t), \mathbf{X}, t) + \mathbf{F}^{\mathrm{self}}(\langle f(\mathbf{X},t)\rangle_{\mathfrak{M}}, \mathbf{X}, t)$$

The matrix form of ODE's

$$d\mathbf{X}/dt = \mathbf{F}(\mathbf{X},t),\ \mathbf{F}(0,t) \equiv 0 \longrightarrow \frac{d\mathbf{X}}{dt} = \sum_{k=1}^{\infty} \mathbb{P}^{1k}\mathbf{X}^{[k]} = \sum_{k=0}^{\infty} \frac{\partial^k \mathbf{F}(0,t)}{\partial \mathbf{X}^k}\frac{\mathbf{X}^k}{(k)!}$$

Kronecker product

$$\mathbf{X}^{[k]} = \underbrace{\mathbf{X}\otimes\ldots\otimes\mathbf{X}}_{k\text{-times}}. \qquad \frac{d\mathbf{X}^{[k]}}{dt} = \sum_{k=0}^{k}\mathbf{X}^{[j]}\otimes\frac{d\mathbf{X}}{dt}\otimes\mathbf{X}^{[k-j-1]} = \sum_{k=1}^{\infty}\sum_{j=0}^{k}\mathbf{X}^{[j]}\otimes\mathbb{P}^{1k}\otimes\mathbf{X}^{[k]}.$$

$$\mathbb{P}^{kj} = \mathbb{P}^{1\,(j-k+1)} \oplus \mathbb{P}^{(k-1)\,(j-1)}, \quad j \geq k,$$

$$\mathbb{P}^{k\,k} = \mathbb{P}^{1\,1} \oplus \mathbb{P}^{(k-1)\,(k-1)} = \left(\mathbb{P}^{11}\right)^{\oplus k}, \quad k \geq 2.$$

$$\frac{d\mathbf{X}^{[k]}}{dt} = \sum_{j=k}^{\infty}\mathbb{P}^{kj}\mathbf{X}^{[j]}$$

$$\frac{d\mathbf{X}^{\infty}}{dt} = \mathbb{P}^{\infty}(t)\mathbf{X}^{\infty} \qquad \mathbb{P}^{\infty} = \begin{pmatrix} \mathbb{P}^{11} & \mathbb{P}^{12} & \ldots & \mathbb{P}^{1k} & \ldots \\ \mathbb{O} & \mathbb{P}^{22} & \ldots & \mathbb{P}^{2k} & \ldots \\ \vdots & \vdots & \ddots & \vdots & \ddots \\ \mathbb{O} & \mathbb{O} & \ldots & \mathbb{P}^{2k} & \ldots \\ \vdots & \vdots & \ddots & \vdots & \ddots \end{pmatrix}$$

The matrix presentation of ODE's solutions

$$\mathbf{X}^{\infty} = \mathbb{R}^{\infty}(t)\mathbf{X}_0^{\infty} \quad \Longleftrightarrow \quad \mathbf{X}(t) = \sum_{k=1}^{\infty} \mathbb{R}^{1k}(t|t_0)\mathbf{X}_0^{[k]}$$

$$\mathbb{R}^{ik}(t|t_0) = \sum_{j=i+1}^{k} \int_{t_0}^{t} \mathbb{R}^{ii}(t|\tau)\mathbb{P}^{ij}(\tau)\mathbb{R}^{jk}(\tau|t_0)d\tau, \quad \mathbb{R}^{ii}(t|t_0) = \left(\mathbb{R}^{11}(t|t_0)\right)^{[i]}$$

$$(\mathbb{R}^{\infty})^{-1} = \mathbb{T}^{\infty} = \begin{pmatrix} \mathbb{T}^{11} & \mathbb{T}^{12} & \dots & \mathbb{T}^{1k} & \dots \\ \mathbb{O} & \mathbb{T}^{22} & \dots & \mathbb{T}^{2k} & \dots \\ \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \mathbb{T}^{kk} & \dots \\ \dots & \dots & \dots & \dots & \dots \end{pmatrix}$$

$$\mathbb{T}^{kk} = \left(\mathbb{R}^{kk}\right)^{-1} = \left(\mathbb{R}^{11}\right)^{-[k]} = \left(\left(\mathbb{R}^{11}\right)^{-1}\right)^{[k]},$$

$$\mathbb{T}^{ik} = -\sum_{l=i}^{k-i} \mathbb{T}^{il}\mathbb{R}^{lk}\mathbb{T}^{kk}, \quad i < k.$$

There can be used also another formulae for $\mathbb{R}^{1k}(t|t_0)$ - matrices evaluation,

which have some more complicate forms, but with more rapid convergence of the corresponding series.

The matrix presentation using Lie algebraic tools

According to the well known Lie algebraic tools[1] the our motion equations can be written using so called Lie map (an evolution operator in the exponential form)

$$\frac{d\mathcal{M}(t|t_0)}{dt} = \mathcal{V}(t) \circ \mathcal{M}(t|t_0),$$ **with the initial condition** $\mathcal{M}(t_0|t_0) = \mathcal{I}d \quad \forall\, t_0 \in \mathfrak{T}$

where $\mathcal{V}(t) = \mathcal{L}_{\mathbf{F}} = \mathbf{F}^*(\mathbf{X})\frac{\partial}{\partial \mathbf{X}} = \sum_{k=0}^{\infty}\left(\mathbf{X}^{[k]}\right)^*(\mathbf{F}_k)^*\frac{\partial}{\partial \mathbf{X}} = \sum_{k=0}^{\infty}\mathcal{L}_{\mathbf{F}}^k$ **is a Lie operator.**

The solution the operator equation can be written in the form of chronological ordered series (Volterra series)

$$\mathcal{M}(t|t_0) = \mathcal{I}d + \sum_{k=1}^{\infty}\int_{t_0}^{t}\int_{t_0}^{\tau_1}\ldots\int_{t_0}^{\tau_{k-1}}\mathcal{V}(\tau_k)\circ\mathcal{V}(\tau_{k-1})\circ\ldots\circ\mathcal{V}(\tau_1)\,d\tau_k\ldots d\tau_1$$

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1 See, for example, A.J.Dragt *Lie Methods for Nonlinear Dynamics with Applications to Accelerator Physics*. University of Maryland, College Park. www.physics.umd.edu/dsat/.

The matrix presentation using Lie algebraic tools
Magnus presentation

The chronological series is not convenient for practical computation. Instead of this series there is used so called Magnus presentation for Lie map

$$\mathcal{M}(t|t_0) = \exp \mathcal{W}(t|t_0; \mathcal{V})$$

$$\mathcal{W}(t|t_0) = \int_{t_0}^{t} \mathcal{V}(\tau)d\tau + \alpha_1 \int_{t_0}^{t} \left\{ \mathcal{V}(\tau), \int_{t_0}^{\tau} \mathcal{V}(\tau') \right\} d\tau +$$

$$+ \alpha_1^2 \int_{t_0}^{t} \left\{ \mathcal{V}(\tau), \int_{t_0}^{\tau} \left\{ \mathcal{V}(\tau'), \int_{t_0}^{\tau'} \mathcal{V}(\tau'')d\tau'' \right\} d\tau' \right\} d\tau +$$

$$+ \alpha_1\alpha_2 \int_{t_0}^{t} \left\{ \left\{ \mathcal{V}(\tau), \int_{t_0}^{\tau} \mathcal{V}(\tau')d\tau' \right\}, \int_{t_0}^{\tau} \mathcal{V}(\tau')d\tau' \right\} d\tau + \dots$$

Here is a commutator for any two operators. Similar formulae can be evaluated up to any order.

The matrix presentation using Lie algebraic tools – Magnus presentation

One can introduce the following presentation for a new operator

$$\mathcal{W}_\lambda(t|t_0;\mathcal{V}) = \sum_{k=1}^{\infty} \lambda^k \mathcal{W}_k(t|t_0;\mathcal{V})$$

After some transformation we can obtain the following family of equalities:

$$\mathcal{W}_1(t|t_0;\mathcal{V}) = \int_{t_0}^{t} \mathcal{V}(\tau)d\tau,$$

$$\mathcal{W}_2(t|t_0;\mathcal{V}) = -\frac{1}{2}\int_{t_0}^{t}\int_{t_0}^{\tau} \left\{\mathcal{V}(\tau),\mathcal{V}(\tau')\right\} d\tau' d\tau.$$

$$\mathcal{W}_3(t|t_0;\mathcal{V}) = \frac{1}{6}\int_{t_0}^{t}\int_{t_0}^{\tau}\int_{t_0}^{\tau'} \left(\left\{\left\{\mathcal{V}(\tau),\mathcal{V}(\tau')\right\},\mathcal{V}(\tau'')\right\} + \right.$$

$$\left. + \left\{\left\{\mathcal{V}(\tau''),\mathcal{V}(\tau')\right\},\mathcal{V}(\tau)\right\}\right) d\tau'' d\tau' d\tau.$$ **and so on.**

The matrix presentation using Lie algebraic tools
Hamiltonian formalism

In the case of Hamiltonian motion equation we can write $\dfrac{d\mathbf{X}}{dt} = \mathbb{J}(\mathbf{X})\dfrac{\partial \mathcal{H}(\mathbf{X},t)}{\partial \mathbf{X}}$, **where**

$$\mathcal{H} = \sum_{k=2}^{\infty} \mathbf{H}_k^*(t)\mathbf{X}^{[k]} = -(1+hx)\frac{q}{\mathcal{E}_0}A_s -$$
$$-(1+hx)\left[(1+\eta)^2 - \left(\frac{m_0c^2}{\mathcal{E}_0}\right)^2 - \left(P_x - \frac{q}{c}A_x\right)^2 - \left(P_y - \frac{q}{c}A_y\right)^2\right]^{1/2}$$

Than one can write $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1 + \mathcal{H}_2 + \sum\limits_{k=3}^{\infty} \varepsilon^{k-2}\mathcal{H}_k$, **where** $\mathcal{H}_k$ **are homogeneous polynomials of *k*-th order. Here** $\mathbf{H}_k(t)$ **- vectors of coefficients for these polynomials.**

This decomposition leads to expansion for motion equation of the corresponding series in according Dragt's approach. After this one can write

$$\mathcal{M}\left(t|t_0; \sum_{k=1}^{\infty} \mathcal{L}_{\mathbf{F}_k}\right) = \ldots \circ \mathcal{M}\left(t|t_0; \mathcal{L}_{\mathbf{G}_k}\right) \circ \mathcal{M}\left(t|t_0; \mathcal{L}_{\mathbf{G}_{k-1}}\right) \circ \ldots$$
$$\ldots \circ \mathcal{M}\left(t|t_0; \mathcal{L}_{\mathbf{G}_2}\right) \circ \mathcal{M}\left(t|t_0; \mathcal{L}_{\mathbf{G}_1}\right),$$

The convergence problem for the matrix formalism

Magnus presentation

We can note the (according to the Ado lemma) every finite-dimensional algebra has faithful finite-dimensional representation. This allows us to use matrix algebras Lie. Using the above mentioned presentations we can obtain the following operator estimation for previous series. For example,

$$\mathcal{W}(t|t_0) = \int_{t_0}^{t} \mathcal{A}(\tau)d\tau + \alpha_1 \int_{t_0}^{t} \left\{ \mathcal{A}(\tau), \int_{t_0}^{\tau} \mathcal{A}(\tau')d\tau' \right\} d\tau + \alpha_1^2 \int_{t_0}^{t} \left\{ \mathcal{A}(\tau), \int_{t_0}^{\tau} \left\{ \mathcal{A}(\tau'), \int_{t_0}^{\tau'} \mathcal{A}(\tau'')d\tau'' \right\} d\tau' \right\} d\tau +$$
$$+ \alpha_1\alpha_2 \int_{t_0}^{t} \left\{ \left\{ \mathcal{A}(\tau), \int_{t_0}^{\tau} \mathcal{A}(\tau')d\tau' \right\}, \int_{t_0}^{\tau} \mathcal{A}(\tau')d\tau'' \right\} d\tau + \ldots$$

Whence it follows

$$\|\mathcal{W}(t|t_0)\| \leq A(t) \left(1 + 2|\alpha_1|A(t) + 4A^2(t)C_2 + 8A^3(t)C_3 + \sum_{l\geq 4} \left(2A(t)\right)^l C_l \right),$$

where

$$A(t) = \int_{t_0}^{t} \|\mathcal{A}(\tau)\| d\tau$$

The convergence problem for the matrix formalism Magnus presentation

Here $C_{2l} = \alpha_{2l} + C_{2l-2}C_{2l-4}$, $C_{2l+1} = \alpha_{2l} + C_3 C_{2l-1}$, $l \geq 2$, $C_0 = 1$, $C_1 = 1$, $C_2 = \alpha_1^2 + |\alpha_1|$, $C_3 = \alpha_1^3 + 2|\alpha_1|$. Let be $\mathcal{W} = \sum_{k>0} \mathcal{W}^k$, where $\mathcal{W}^k$ enclose all k nested Lie brackets. Then we

Have the following inequality $\|\mathcal{W}^k(t|t_0)\| \leq A(t)\,(2A(t))^k\, C_k,\quad k \geq 0$, and for coefficients α_{2k} we have

$$|\alpha_{2m}| \leq \frac{2}{(2\pi)^{2m}} \sum_{k\geq 1} \frac{1}{2^{2k}} < \frac{4}{(2\pi)^{2m}}.$$

Let be $M = \int\limits_{t_0}^{T_2} A(\tau)d\tau$, then $\|\mathcal{W}^k\|_{L_1} \leq 2^k M^{k+1} C^k$ for all sufficiently great k. The majorant

series with general members $2^k M^{k+1} C_k$ will be converge (according to D'Alember criterion) if there hold the following inequality

$$\lim_{k\to\infty} \frac{2^{k+1}M^{k+2}C_{k+1}}{2^k M^{k+1} C_k} = q < 1.$$

For $k = 2l$,

$$q = 2M \lim_{l\to\infty} \frac{C_{2l+1}}{C_{2l}} = 2M \lim_{l\to\infty} \frac{\alpha_{2l} + C_3 C_{2l-1}}{\alpha_{2l} + C_{2l-2}C_{2l-4}} = 2M.$$

So the majorizing series will converge on the assumption of $M < 1/2$. Therefore our series will converge absolutely.

The convergence problem for the matrix formalism

We can derive corresponding conditions for convergence of matrix formalism for ODE's. Let cite corresponding estimations.

Let be $\dfrac{d\mathbf{X}}{dt} = \sum_{k=1}^{\infty} \mathbb{P}^{1k}\mathbf{X}^{[k]}$**, from where** $\mathbf{X}(t) = \sum_{k=1}^{\infty} \mathbb{R}^{1k}(t|t_0)\mathbf{X}_0^{[k]}$ **and we have** $\|\mathbf{X}_0\| \leq r$ **,**

and $\|\dfrac{\partial^k \mathbf{F}(\mathbf{X},\mathbf{U},t)}{\partial x_1^{k_1}\ldots x_n^{k_n}}\| \leq \varphi(t)$**,** $M = \int_{\mathcal{T}} \varphi(t)dt, \; L = \sup_{t,\tau\in\mathcal{T}} \|\mathbb{R}^{11}(t,\tau)\|$. **We can show that**

there are the next inequalities $\sup_{t,\tau\in\mathcal{T}} \|\mathbb{R}^{ij}(t,\tau)\| \leq jL^j$ **and** $\|\mathbb{P}^{ij}(t)\| \leq \dfrac{\varphi(t)}{(j-1)!}$.

Let be $J_i(L,M) = \begin{cases} \prod_{k=3}^{i} \left\{ \frac{L^{k-1}M(k-1)}{(k-2)!} + 1 \right\}, i \geq 3, \\ 1, i = 2 \end{cases}$ **then we have (** $\overline{\mathbf{X}}$ **is an exact solution):**

$$\|\overline{\mathbf{X}} - \mathbf{X}_N\| \leq \sum_{k=N+1}^{\infty} \frac{r^k L^{k+1} M k}{(k-1)!} J_k(L,M).$$

Some examples for truncated series for solutions

Let consider some example of matrix expansion for a particular case of the Lie map

$$\mathcal{L}_{\mathbf{G}_m} \circ \mathbf{X} = \mathbb{G}_m \mathbf{X}^{[m]}, \;\; (\mathcal{L}_{\mathbf{G}_m})^2 \circ \mathbf{X} = \mathcal{L}_{\mathbf{G}_m} \circ \mathbb{G}_m \mathbf{X}^{[m]} = \mathbb{G}_m \mathcal{L}_{\mathbf{G}_m} \circ \mathbf{X}^{[m]} = \mathbb{G}_m \mathbb{G}_m^{\oplus m} \mathbf{X}^{[2m-1]}, \ldots$$

Then we can obtain

$$\exp\left(\mathcal{L}_{\mathbf{G}_m}\right) \circ \mathbf{X} = \mathbf{X} + \sum_{k=1}^{\infty} \frac{\mathbb{P}_m^{k\,1}}{k!} \mathbf{X}^{[k(m-1)+1]},$$

where $\mathbb{P}_m^{k\,1} = \prod_{j=1}^{k} \mathbb{G}_m^{\oplus((j-1)(m-1)+1)}$**, then we can write**

$$\mathcal{M}_{\leq 3} \circ \mathbf{X} = \mathbb{M}^{11} \left(\mathbf{X} + \sum_{m=2}^{3} \sum_{k=1}^{\infty} \frac{\mathbb{P}_m^{k1}}{k!} \mathbf{X}^{[k(m-1)+1]} + \sum_{l=1}^{\infty} \sum_{k=1}^{\infty} \frac{1}{k!l!} \mathbb{P}_2^{kl}\, \mathbb{P}_3^{l\,(k+1)}\, \mathbf{X}^{[2l+k+1]} \right).$$

here we introduce the following notation $\mathcal{M}_{\leq k} = \mathcal{M}_k \circ \mathcal{M}_{k-1} \circ \ldots \circ \mathcal{M}_2 \circ \mathcal{M}_1$

The expansions similar to the previous expression allows us to evaluate the necessary map up to desired order. It should be noted that corresponding evaluation procedures can be realized both in symbolic and numerical forms.

The preservation of qualitative properties in matrix formalism (qualitative properties)

Usually in beam physics there is used the Hamiltonian formalism for particle beam motion description. This automatically leads us to following equalities $\frac{d\mathbf{X}}{dt} = \mathbb{J}(\mathbf{X})\frac{\partial \mathcal{H}(\mathbf{X},t)}{\partial \mathbf{X}}$, were $\mathbb{J}(\mathbf{X})$ is a symplectic matrix $2n \times 2n$, for example $\mathbb{J}(\mathbf{X}) = \mathbb{J}_0 = \begin{pmatrix} \mathbb{O} & \mathbb{E} \\ -\mathbb{E} & \mathbb{O} \end{pmatrix}$.

The Jacobi matrix $\mathbb{M}(\mathbf{X}, t \,|\, t_0; \mathcal{M}) = \mathbb{M}(\mathbf{X}; t \,|\, t_0) = \frac{\partial \mathcal{M}(t \,|\, t_0; \mathcal{H}) \circ \mathbf{X}}{\partial \mathbf{X}^*}$ satisfies to the following symplecticity condition $\mathbb{M}^*(\mathbf{X}; t \,|\, t_0)\mathbb{J}(\mathbf{X})\mathbb{M}(\mathbf{X}; t \,|\, t_0) = \mathbb{J}(\mathbf{X})$. Here we have $\det \mathbb{M}(\mathbf{X}; t \,|\, t_0) \equiv 1$.
According to the matrix formalism one can derive

$$\mathbb{M}(\mathbf{X}; t \,|\, t_0) = \frac{\partial \mathcal{M}(t \,|\, t_0; \mathcal{H}) \circ \mathbf{X}}{\partial \mathbf{X}^*} = \sum_{k=1}^{\infty} \mathbb{R}^{1k}(t \,|\, t_0; \mathcal{H}) \frac{\partial \mathbf{X}^{[k]}}{\partial \mathbf{X}^*}. \quad (1)$$

Using the Kronecker product and sum properties we can derive

$$\mathbb{M}(\mathbf{X}; t \,|\, t_0) = \sum_{k=1}^{\infty} \sum_{j=0}^{k-1} \mathbb{R}^{1k}(t \,|\, t_0; \mathcal{H}) \mathbf{X}^{[j]} \otimes \mathbf{E}_{2n} \otimes \mathbf{X}^{[k-j-1]}. \quad (2)$$

The preservation of qualitative properties in matrix formalism (qualitative properties)

Replacing (2) into (1) one can derive $\mathbb{M}(\mathbf{X};t\,|\,t_0) = \sum_{k=1}^{\infty}\sum_{j=0}^{k-1}\mathbb{R}^{1k}(t\,|\,t_0;\mathcal{H})\,\mathbf{X}^{[j]}\otimes\mathbb{E}\otimes\mathbf{X}^{[k-j-1]}.$ **From here we can describe**

$$\underbrace{\left(\mathbb{R}^{11}\right)^*\mathbb{J}_0\mathbb{R}^{11}}_{k=l=1} + \underbrace{\left(\mathbf{X}\otimes\mathbb{E}+\mathbb{E}\otimes\mathbf{X}\right)^*\left(\mathbb{R}^{12}\right)^*\mathbb{J}_0\mathbb{R}^{11}}_{k=2,\ l=1} +$$
$$+\underbrace{\left(\mathbb{R}^{11}\right)^*\mathbb{J}_0\mathbb{R}^{12}\left(\mathbf{X}\otimes\mathbb{E}+\mathbb{E}\otimes\mathbf{X}\right)}_{k=1,\ l=2} + \sum_{\substack{k,l=1\\k+l>3}}^{\infty}\left(\mathbf{X}^{\odot k}\right)^*\left(\mathbb{R}^{1k}\right)^*\mathbb{J}_0\mathbf{X}^{\odot l} = \mathbb{J}_0,$$

were $\mathbf{X}^{\odot(k-1)} = \sum_{j=0}^{k-1}\mathbf{X}^{[j]}\otimes\mathbb{E}\otimes\mathbf{X}^{[k-j-1]}.$ **Denoting** $\mathbb{R}^{1k} = \mathbb{R}^{11}\mathbb{Q}^{1k}$ **(here** $\mathbb{Q}^{11} = \mathbb{E}$ **) we derive**

$$\sum_{k+l=m}\left(\mathbf{X}^{\odot k}\right)^*\left(\mathbb{Q}^{1\,(k+1)}\right)^*\mathbb{J}_0\mathbb{Q}^{1\,(l+1)}\mathbf{X}^{\odot l} = 0, \quad m\geq 1.$$

Or the following equalities sequence

$$\begin{gathered}\left(\mathbf{X}^{\odot 1}\right)^*\left(\mathbb{Q}^{12}\right)^*\mathbb{J}_0 + \mathbb{J}_0\mathbb{Q}^{12}\mathbf{X}^{\odot 1} = 0,\\ \left(\mathbf{X}^{\odot 2}\right)^*\left(\mathbb{Q}^{13}\right)^*\mathbb{J}_0 + \left(\mathbf{X}^{\odot 1}\right)^*\left(\mathbb{Q}^{12}\right)^*\mathbb{J}_0\mathbb{Q}^{12}\mathbf{X}^{\odot 1} + \mathbb{J}_0\mathbb{Q}^{13}\mathbf{X}^{\odot 2} = 0, \qquad \textbf{(3)}\\ \left(\mathbf{X}^{\odot 3}\right)^*\left(\mathbb{Q}^{14}\right)^*\mathbb{J}_0 + \left(\mathbf{X}^{\odot 2}\right)^*\left(\mathbb{Q}^{13}\right)^*\mathbb{J}_0\mathbb{Q}^{12}\mathbf{X}^{\odot 1} +\\ + \left(\mathbf{X}^{\odot 1}\right)^*\left(\mathbb{Q}^{12}\right)^*\mathbb{J}_0\mathbb{Q}^{13}\mathbf{X}^{\odot 2} + \mathbb{J}_0\mathbb{Q}^{14}\mathbf{X}^{\odot 3} = 0, \ \ldots\end{gathered}$$

The preservation of qualitative properties in matrix formalism (qualitative properties)

The equalities sequences (3) can be solved step-by-step both in analytical and in numerical modes. It should be noted that these equalities impose simple algebraic conditions on corresponding matrix elements. These equalities have the form of linear algebraic equalities with integer coefficients! For example, for four dimensional phase space for the second order matrix $\mathbb{Q}^{[2]} = \{q_{ij}\}$ we obtain

$$\mathbb{Q}^{12} = \begin{bmatrix} q_{11} & q_{12} & q_{13} & q_{14} & q_{15} & q_{16} & q_{17} & q_{18} & q_{19} & q_{110} \\ q_{21} & q_{22} & q_{23} & q_{15} & q_{25} & q_{17} & q_{27} & q_{19}/2 & 2\,q_{110} & q_{210} \\ q_{31} & q_{32} & q_{33} & -2\,q_{11} & -2\,q_{21} & -q_{12} & -q_{22} & q_{14}/2 & -q_{15} & q_{25}/2 \\ q_{32}/2 & 2\,q_{33} & q_{43} & -q_{12} & -q_{22} & q_{32}/2 & 2\,q_{33} & q_{43} & -q_{12} & -q_{22} \end{bmatrix}.$$

It should be noted that similar matrices can be precomputed (for example, using Maple or Mathematica packages) and kept that in a special database. This presentation guaranties us fulfilment of the symplecticity conditions up the necessary order for arbitrary interval of independent variable!

The preservation of qualitative properties in matrix formalism (exact solutions)

The correctness of the matrix formalism can be tested for some simple examples.

1. One-dimensional nonlinear equation

$$\frac{dx}{dt} = K_n x^n.$$

The exact solution of this equality has the form

$$x(t) = \sqrt[1-n]{K_n(1-n)(t-t_0) + x_0^{1-n}}.$$

For Lie operator we can write

$$\mathcal{M}(t, t_0) = exp\{(t-t_0)K_n x^n \frac{\partial}{\partial x}\}.$$

!

After some simple calculations one can obtain the desired expression!

$$\mathcal{M} \circ x_0 = x_0 \sum_{k=0}^{\infty} \binom{\frac{1}{1-n}}{k} ((1-n)K_n(t-t_0)x_0^{n-1})^k = \frac{x_0}{\sqrt[n-1]{1+(1-n)K_n(t-t_0)x_0^{n-1}}}$$

The preservation of qualitative properties in matrix formalism (exact solutions)

The correctness of the matrix formalism can be tested for some simple examples.

2. Fractionally rational solution of nonlinear equations.

In some cases we search the solution of the nonlinear equations in the fractionally rational form

$$\mathcal{M} \circ \mathbf{X}_0 = \mathbf{X}\left(\mathbf{X}_0; t \,|\, t_0\right) = \frac{\mathbf{P}_N\left(\mathbf{X}_0; t \,|\, t_0\right)}{Q_L\left(\mathbf{X}_0; t \,|\, t_0\right)},$$

where

$$\mathbf{P}_N\left(\mathbf{X}_0; t \,|\, t_0\right) = \sum_{k=0}^{N} \mathbb{P}^k(t \,|\, t_0)\mathbf{X}_0^{[k]}, \quad Q_L\left(\mathbf{X}_0; t \,|\, t_0\right) = \sum_{j=0}^{L} \left(\mathbf{Q}_j(t \,|\, t_0)\right)^* \mathbf{X}_0^{[j]}.$$

Let consider the next case $\mathcal{M} = \mathcal{M}_m = \exp\left(t - t_0\right)\mathcal{L}_m$, where $\mathcal{L}_m = \mathbf{G}_m^*(\mathbf{X}_0)\partial/\partial\mathbf{X}_0$.

After some calculation one can obtain

$$\mathcal{M}_m \circ \mathbf{X}_0 = \mathbf{X}_0 + \sum_{k=1}^{\infty} \frac{(t - t_0)^k \mathbb{P}_m^{1k}}{k!} \mathbf{X}_0^{[k(m-1)+1]}, \quad \mathbb{P}_m^{1k} = \prod_{j=1}^{k} \mathbb{G}_m^{\oplus((j-1)(m-1)+1)}.$$

Let introduce

$$\mathbb{C}_m^k = \left((t - t_0)/(k - 1)!\right) \mathbb{P}_m^{1\,(k-1)}$$

The preservation of qualitative properties in matrix formalism (exact solutions)

then
$$\mathbb{C}_m^k = \mathbb{P}_m^k - \sum_{j=0}^{L} \mathbf{Q}_j^* \otimes \mathbb{C}_m^{k-j}, \quad 1 \le k \le N,$$
$$\mathbb{C}_m^k + \sum_{j=1} \mathbf{Q}_j^* \otimes \mathbb{C}_m^{k-j} = 0, \quad k > N.$$

For the second order nonlinear Hamiltonian equations

$$\frac{dx}{dt} = ax^2, \quad \frac{dP_x}{dt} = bx^2 - 2axP_x, \tag{4}$$

we can obtain

$$\mathbf{X} = \frac{\mathbf{X}_0 + \mathbb{P}_2^2 \mathbf{X}_0^{[2]} + \mathbb{P}_2^3 \mathbf{X}_0^{[3]} + \mathbb{P}_2^4 \mathbf{X}_0^{[4]}}{1 + \mathbf{Q}_1^* \mathbf{X}_0}. \tag{5}$$

where
$$Q_0 = 1, \quad \mathbf{Q}_1 = -(t - t_0)\begin{pmatrix} a \\ 0 \end{pmatrix}, \quad \mathbb{P}_2^2 = a(t - t_0)\begin{pmatrix} 0 & 0 & 0 \\ -b & 3a & 0 \end{pmatrix},$$

$$\mathbb{P}_2^3 = a(t - t_0)^2 \begin{pmatrix} 0 & 0 & 0 & 0 \\ -b & 3a & 0 & 0 \end{pmatrix}, \quad \mathbb{P}_2^4 = \frac{a^2 (t - t_0)^3}{3}\begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ -b & 3a & 0 & 0 & 0 \end{pmatrix}.$$

We should note that (5) is exact solution of the equation system (4)!

The preservation of qualitative properties in matrix formalism (energy conservation)

It is known that in general cases the symplecticity of the map (exact or approximate map) does not guarantee the energy conservation. That is why we should additionally constrain the used approximated map. In another words on the every step we must guarantee the energy conservation low, which can be written in the following forms

$$E(\mathbf{Q},\mathbf{P},t_k) = E(\mathbf{Q},\mathbf{P},t_{k-1}),\ \forall k \geq 1, \mathbf{X} = \begin{pmatrix}\mathbf{Q}\\ \mathbf{P}\end{pmatrix}, \qquad \mathcal{M}(t_k|t_{k-1}) \circ E(\mathbf{X},t_k) \equiv E(\mathbf{X},t_{k-1}).$$

These conditions can be realized using some correction procedure. We demonstrate this process using the matrix formalism

$$\mathcal{M}(t_k|t_{k-1}) \circ E(\mathbf{X},t_k) = E(\mathcal{M}(t_k|t_{k-1}) \circ \mathbf{X}, t_{k-1})) = E\left(\sum^{\infty} \mathbb{R}^{[1j]}(t_k|t_{k-1})\mathbf{X}^{[j]}\right)$$

For linear case we have $E(\mathbf{Q}_{k-1},\mathbf{P}_{k-1},t_{k-1}) = \frac{1}{2}\left(\mathbf{X}^{\mathrm{T}}(t_{k-1}) \cdot \mathbb{A} \cdot \mathbf{X}_{k-1}(t_{k-1}))\right), \mathbb{A} = \begin{pmatrix} 0 & 1 \\ -\omega^2 & 0\end{pmatrix}$

$$E\left(\mathbb{R}^{[11]}(t_k|t_{k-1})\mathbf{X}_{k-1}\right) = \left(\mathbf{X}_{k-1}^{\mathrm{T}}\left(\mathbb{R}_k^{[11]}\right)^{\mathrm{T}} \cdot \mathbb{A} \cdot \mathbb{R}_k^{[11]}\mathbf{X}_{k-1}\right) = \left(\mathbf{X}_k^{\mathrm{T}} \cdot \mathbb{A} \cdot \mathbf{X}_k\right) = \left(\mathbf{X}_{k-1}^{\mathrm{T}} \cdot \mathbb{A} \cdot \mathbf{X}_{k-1}\right)$$

where $\mathbb{R}_k^{[11]} = \mathbb{R}^{[11]}(t_k|t_{k-1})$, and we have $E_k = E_{k-1}$!

The preservation of qualitative properties in matrix formalism (energy conservation)

Similar evaluation for nonlinear Hamiltonian and using full "matrix map" $\sum_{j=1}^{\infty} \mathbb{R}^{[1j]}(t_k|t_{k-1})\mathbf{X}^{[j]}$ leads us to the same result. On the practice we apply some truncated transformation of *N*-th order $\sum_{j=1}^{N} \mathbb{R}^{[1j]}(t_k|t_{k-1})\mathbf{X}^{[j]}$ and similar transformation doesn't conserve nonlinear Hamiltonian!

There is a problem: Can we construct an integration scheme that is both symplectic and energy-conserving properties for a broad class of Hamiltonian systems? The well known Zhang and Marsden theorem answer – in general case – NO!

If we want to conserve nonlinear Hamiltonian, than we should "correct a little" our truncated matrix map. In another words, some elements of $\mathbb{R}^{[1j]}(t_k|t_{k-1})$ we should be corrected.

For this purpose we can evaluate some equations (see, an example, the correction procedure for symplectification). Here there are some different approaches. The choice of appropriate variant depends on the practical problem: the symplectification condition is universal property, while the energy conservation depends on the energy function (Hamiltonian)!

Conclusion

1. The basic principal difference the matrix formalism for presentation of motion equations in the form of ODE's or Hamiltonian equations: we handle with **two dimensional matrices** instead of multidimensional tensors, similar in MAD, Transport, COSY Infinity and so on.
2. The matrix formalism can be used for different models of beam dynamics (in the frame of the successive approximations approach), **including space charge forces**.
   The "improvement" of corresponding models is realized using step-by-step process (both increasing of approximation order and variation of corresponding matrices).
3. Linear and "nonlinear" matrices can be evaluated both in **symbolic** (and to keep in special data bases) and in **numerical forms** (using appropriate numerical methods, for example, symplectic Runge-Kutta method or others for corresponding matrix ODE's).
4. The matrix formalism **can be symplectified** with comparative ease. Also we can **compute approximate invariants** for particle beams.
5. The matrix formalism permits different correction procedures for **energy conservation**.
6. The matrix formalism is compatible with optimization procedures of beam dynamics. For this purpose we can use only corresponding matrix elements.
7. The matrix formalism admit **numerical code parallelization and distribution** (including Grid- and Cloud technologies) naturally.
8. The matrix formalism can be easily embedded into **the Virtual Accelerator concept**.

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