

# SELF-CONSISTENT TRANSFER MAPS FOR HIGH INTENSITY BEAMS

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# OUTLINE

- Transfer maps in general
  - Single-particle maps
  - Space charge maps
    - The 3 pillars of potential computation:
      - Differential Algebra
      - Duffy transformation
      - Distribution reconstruction from moments
    - Kick map

#### MATHEMATICAL MODEL OF PERIODIC ACCELERATORS



# **POISSON EQUATION**

$$\Delta \Phi = -\frac{\rho}{\varepsilon}, \quad \text{in } V$$
  
subject to  $B\left(\Phi|_{\partial V}, \frac{\partial \Phi}{\partial n}|_{\partial V}\right) = 0$   
Decompose:  $\Phi = \Phi_1 + \Phi_2$   
Free space solution: Laplace equation:  
 $\Phi_1(\vec{r}) = \frac{1}{4\pi} \int_V \frac{\rho\left(\vec{r'}\right)}{\left\|\vec{r} - \vec{r'}\right\|} dV \quad B_m\left(\Phi|_{\partial V}, \frac{\partial \Phi}{\partial n}|_{\partial V}, \Phi_1|_{\partial V}\right) = 0$ 

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Free space solution:  
$$\Phi_1\left(\vec{r}\right) = \frac{1}{4\pi} \int_V \frac{\rho\left(\vec{r'}\right)}{\left\|\vec{r} - \vec{r'}\right\|} dV$$
  
 $B_m\left(\Phi|_{\partial V}, \frac{\partial \Phi}{\partial n}|_{\partial V}, \Phi_1|_{\partial V}\right) = 0$ 

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# **FREE SPACE SOLUTIONS**

2D free space solution:

3D free space solution:

$$\Phi_1\left(\vec{r}\right) = \frac{1}{2\pi} \int_S \rho\left(\vec{r'}\right) \ln\|\vec{r} - \vec{r'}\| dS \quad \Phi_1\left(\vec{r}\right) = \frac{1}{4\pi} \int_V \frac{\rho\left(r'\right)}{\left\|\vec{r} - \vec{r'}\right\|} dV$$

- Singular integrals
- Theory says that the potential should be analytic in V if the charge density distribution is analytic in V
- Evaluation of integrals by standard methods is problematic
- Even if some clever integration method is used that avoids the singularity problem, the convergence radius of the resulting Taylor expansion of the potential tends to zero
- Need to perform integrations in DA
- Need straightforward method to control accuracy
- Must have large convergence region

# **RECASTING THE INTEGRALS**

- The multiple integrals are considered as iterated integrals
- Each integral is rewritten as an initial value problem
- Example:

To evaluate 
$$I(a, b; p) = \int_{a}^{b} f(y; p) dy$$
  
Define  $g(x; p) = \int_{a}^{x} f(y; p) dy$   
It follows that  $\frac{dg(x; p)}{dx} = f(x; p), \quad g(a; p) = 0$   
Hence  $I(a, b; p) = g(b; p)$ 

- Solve initial value problem using *DA integrators (we use 8<sup>th</sup> order RK with 7<sup>th</sup> order automatic step size control)*
- Gives not just the value of the integral, but also the *Taylor* expansion of the integral around an arbitrary parameter value p of the function f
- Accuracy can be controlled not just for the integrals' values, but also their derivatives w.r.t. parameters (in RK8 can be set a priori)

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- A coordinate transformation that removes the singularity through the Jacobian of the transformation; works in both 2D and 3D
- The following steps are performed:
  - Split the integral over the whole domain into sum of integrals over boxes such that the singularity is at the lower left corner of each box
  - Then, split each box into 2 triangles (2D) or 3 pyramids (3D)
  - Apply the special coordinate transformation to each triangle/pyramid that removes the singularity
  - This is done by remapping each triangle/pyramid into a (different) square/cube)
- Resulting integrals can be done by standard methods (Runge-Kutta for example)
- Sum up all boxes
- Do everything in DA; result is the Taylor expansion of the potential around a point (typically the reference particle)

• Start with a box large enough (of course this also includes the support of the charge distribution function)

• The cross corresponds to the location of the reference particle

• Then, this is the integration region, and the result should be the Taylor expansion of the potential around the cross

• Ideally, the convergence region should be at least as large as the box



# DUFFY TRANSFORMATION FOR UNIFORM SQUARE



$$\int_{a}^{b} \int_{a}^{b} \ln(\sqrt{(x-x_0)^2 + (y-y_0)^2}) dx dy$$

$$\int_{c}^{y_{0}x_{0}} \int \ln(\sqrt{(x-x_{0})^{2} + (y-y_{0})^{2}}) dx dy$$

$$+ \int_{c}^{y_{0}} \int \ln(\sqrt{(x-x_{0})^{2} + (y-y_{0})^{2}}) dx dy$$

$$+ \int_{y_{0}}^{d} \int \ln(\sqrt{(x-x_{0})^{2} + (y-y_{0})^{2}}) dx dy$$

$$+ \int \int \int \ln(\sqrt{(x-x_{0})^{2} + (y-y_{0})^{2}}) dx dy$$

$$= \int_{y_{0}x_{0}}^{a} \ln(\sqrt{(x-x_{0})^{2} + (y-y_{0})^{2}}) dx dy$$

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$$u_{1} = \frac{x - x_{0}}{b - x_{0}}; u_{2} = \frac{y - y_{0}}{d - y_{0}};$$
$$\lambda_{1}\lambda_{2} \int_{0}^{1} \int_{0}^{1} \ln(\sqrt{(\lambda_{1}u_{1})^{2} + (\lambda_{2}u_{2})^{2}}) du_{1} du_{2};$$
$$\lambda_{1} = b - x_{0}; \lambda_{2} = d - y_{0}$$





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$$w_{1} = u_{1}; w_{2} = \frac{u_{2}}{u_{1}}$$

$$\lambda_{1}\lambda_{2}\int_{0}^{1}\int_{0}^{1}w_{1}\ln(\lambda_{1}^{2}w_{1}^{2} + \lambda_{2}^{2}w_{1}^{2}w_{2}^{2})dw_{1}dw_{2}$$

$$= \lambda_{1}\lambda_{2}\int_{0}^{1}\int_{0}^{1}w_{1}\ln(\lambda_{1}^{2} + \lambda_{2}^{2}w_{2}^{2})dw_{1}dw_{2}$$
SINGULARITY REMOVED!



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- After performing each integration in DA and summing up the values (8 in 2D and 24 in 3D) the Taylor expansion is obtained
- It goes through exactly the same way if the uniform distribution is replaced with any analytic distribution function
- Hence, if the distribution is given analytically, the method produces the Taylor expansion of the potential around the reference orbit
- The reference particle's orbit may or may not coincide with the beam centroid



# **3D EXAMPLE 1: UNIFORM SPHERE (KV)**

Computed potential as taylor expansion				
I	COEFFICIENT	ORDER	EXPON	ENTS
			ху	Z
1	0.4996370018951680	0	0 0	0
2	1666657104620803	2	2 0	0
3	1666657104620803	2	02	0
4	1666657104620802	2	0 0	2
5	1725493873288436E-0	3 4	4 0	0
6	0.5195757808234870E-0	3 4	2 2	0
7	1725493873286667E-0	3 4	04	0
8	0.5195757808445904E-0	3 4	2 0	2
9	0.5195757808421458E-0	3 4	02	2
10	1725493873298274E-0	3 4	0 0	4
11	2820031064842127E-0	6 04	6 0	0
12	0.2455499056204024E-0	6 3	4 2	0
13	0.2457695373273448E-0	3 6	24	0
14	2820031076101128E-0	6 04	06	0
15	0.2457695389517980E-0	3 6	4 0	2
16	2824987224553016E-0	6 2	2 2	2
17	0.2455499050171186E-0	3 6	04	2
18	0.2455499067282470E-0	3 6	2 0	4
19	0.2457695382008953E-0	3 6	02	4
20	2820031054867415E-0	6 04	0 0	6



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### **3D EXAMPLE 2: UNIFORM BOX**

Computed potential as taylor expansion				
I	COEFFICIENT	ORDER	EXPO	NENTS
			х у	Z
1	0.7576021548382070	0	0 0	0
2	1666666666209941	2	2 0	0
3	1666666666209941	2	0 2	0
4	1666666666209941	2	0 0	2
5	2041958853924232E-01	4	4 0	0
6	0.6125876674821989E-01	4	2 2	0
7	2041958853924232E-01	4	04	0
8	0.6125876674821994E-01	4	2 0	2
9	0.6125876674821994E-01	4	02	2
10	2041958853924233E-01	4	0 0	4
11	2836051976365867E-03	6	6 0	0
12	0.2127042457063774E-02	6	4 2	0
13	0.2127041022347797E-02	6	2 4	0
14	2836051976365908E-03	6	0 6	0
15	0.2127041022347805E-02	6	4 0	2
16	2552448368690466E-01	6	2 2	2
17	0.2127042457063789E-02	6	0 4	2
18	0.2127042457063780E-02	6	2 0	4
19	0.2127041022347800E-02	6	0 2	4
20	2836051976365913E-03	6	0 0	6



### **3D EXAMPLE 3: GAUSSIAN**

Computed potential as taylor expansion				
I	COEFFICIENT	ORDER	EXPONENTS	
			ху z	
1	0.1899346134538555	0	0 0 0	
2	2857213616760714	2	200	
3	2857213616760714	2	020	
4	2857213616760714	2	0 0 2	
5	0.3856272870549544	4	4 0 0	
6	0.7717373303298547	4	220	
7	0.3856272870549544	4	040	
8	0.7717373303298548	4	2 0 2	
9	0.7717373303298548	4	0 2 2	
10	0.3856272870549544	4	0 0 4	
11	4132844211752644	6	600	
12	-1.239760030495708	6	4 2 0	
13	-1.239760030851594	6	240	
14	4132844211752643	6	0 6 0	
15	-1.239760030851594	6	4 0 2	
16	-2.480452389375887	6	2 2 2	
17	-1.239760030495708	6	042	
18	-1.239760030495708	6	204	
19	-1.239760030851594	6	024	
20	4132844211752643	6	0 0 6	



# **CONVERGENCE REGION**

- It can be shown that the region of convergence of the multiple Taylor series of the potential is a box with sides equal to the closest boundaries in each spatial direction
- Therefore, it is advantageous to pick the computational box symmetric w.r.t. the expansion point
- According to theory, by rearranging the Taylor series into a sequence of homogeneous polynomials, the convergence region becomes a starshaped region that cannot be smaller than the original convergence region

### **POTENTIAL CONVERGENCE**



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#### **MOMENTS OF THE DISTRIBUTION**

- If the distribution is not known analytically, can it be reconstructed from something?
- Yes, from the moments of the distribution
- <u>Theorem</u>: smooth distribution functions with compact support (and some with non-compact support, such as the Gaussian) are uniquely determined by their moments

#### **MOMENTS OF THE DISTRIBUTION**

- What can be said in the case of a finite set of common moments?
- The distributions sharing a finite set of common moments will resemble each other
- What is the convergence like in the limit of large number of same moments?
- Interestingly, the tail probabilities converge faster!

#### **CONVERGENCE OF THE MOMENT METHOD**

**Theorem 1** Let any two arbitrary distributions  $F(\cdot)$  and  $G(\cdot)$  have the same first 2p moments:  $m_i(F) = m_i(G) = m_i$ , i = 0, 1, 2, ..., 2p with  $m_0 = 1$ . Then, for all values of x,

$$\left|F\left(x
ight)-G\left(x
ight)
ight|\leqrac{1}{\mathbf{V}_{p}^{T}\left(x
ight)\mathbf{M}_{p}^{-1}\mathbf{V}_{p}\left(x
ight)},$$

where  $\mathbf{V}_{p}(x) = \left(1, x, x^{2}, \dots, x^{p}\right)$  and

$$\mathbf{M}_{p} = \begin{pmatrix} 1 & m_{1} & m_{2} & \cdots & m_{p} \\ m_{1} & m_{2} & m_{3} & \cdots & m_{p+1} \\ m_{2} & m_{3} & m_{4} & \cdots & m_{p+2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ m_{p} & m_{p+1} & m_{p+2} & \cdots & m_{2p} \end{pmatrix}$$

Thus, the bound goes to zero at the rate

$$x^{-2p}$$
 as  $x \to \infty$ .

#### DISTRIBUTION RECONSTRUCTION FROM MOMENTS

- Two different approaches:
  - Based on generic function approximation: orthogonal polynomials
  - Based on statistics: method of moments

#### Orthogonal polynomials:

- Compact support and Cartesian coordinates: Jacobi polynomials, moment-based approach
- Take the simplest special case: linear combination of Legendre polynomials
- Minimizes the mean squared error
- Method of moments:
  - Linear combination of monomials
- Both methods: solve for the coefficients by assuming a finite set of moments known
  - this determines the highest degree of the polynomial

#### LEGENDRE POLYNOMIALS

$$\int_{-1}^{1} P_m(x) P_n(x) dx = \frac{2}{2n+1} \delta_{mn}$$

$$\rho(x) = \sum_n C_n P_n(x) \qquad \int_{-1}^{1} P_n(x) \rho(x) dx = C_n \frac{2}{2n+1}$$

$$\int_{-1}^{1} P_n(x) \rho(x) dx = \int_{-1}^{n} \left(\sum_{i=0}^{n} a_i x^i\right) \rho(x) dx = \sum_{i=0}^{n} a_i m_i \qquad \int_{-1}^{1} P_n(x) \rho(x) dx = \sum_i P_n(x_i)$$

$$C_n = \left(2n+1\right) \sum_{i=0}^{n} a_i m_i \qquad C_n = \left(2n+1\right) \sum_{i=0}^{n} P_n(x_i)$$

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#### **METHOD OF MOMENTS**

$$\rho(x) = \sum_{n} C_{n} x^{n}$$

$$m_n = \int x^n \sum_i (C_i x^i) \mathrm{d}x$$

$$\mathbf{T}_{mn} = \int x^{m+n} \mathrm{d}x$$

 $\overrightarrow{M} = \mathbf{T}\overrightarrow{C}$ 

$$\vec{C} = \mathbf{T}^{-1} \vec{M}$$

# T is ill-conditioned, so truncated SVD has to be used for the inversion.

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# WHICH METHOD IS BETTER?

- The matrix to be inverted in the moment method is a Hilbert-like matrix; notoriously difficult to use in numerical computations
- That's why we use truncated SVD inversion, which is stable to at least order 20-25
- Legendre is stable to even higher orders, since there is nothing to invert
- Running times are comparable (excluding preprocessing), with Legendre being somewhat faster
- Therefore, the Legendre method seems to be the better choice

# DISTRIBUTION RECONSTRUCTED FROM 15<sup>th</sup> Order Moments



$$\rho(x) = \frac{e^{-\frac{x^2}{2\sigma_x^2} - \frac{y^2}{2\sigma_y^2}}}{2\pi\sigma_x\sigma_y}, \sigma_x = \sigma_y = \frac{1}{3}$$

#### **OTHER DISTRIBUTIONS**







#### Ideal Potential

#### Calculated Potential

#### Difference (absolute)







# SAMPLE MOMENTS VS. TRUE MOMENTS

- In practice, not only we don't know the analytical distribution, but also we don't know the true moments
- All we have is a finite number of particles from which we can compute a finite set of sample moments
- Replace the true moments with sample moments everywhere
- Does anything change significantly?

### SAMPLE MOMENT CONVERGENCE



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#### **RECONSTRUCTION METHODS REVISITED**

- If sample moments are used instead of true moments, is it still true that Legendre is better?
- Interestingly, not always!
- The reason is that the difference between the true and sample moments can be thought of as an error in the right hand sides of two systems of linear equation that determine the distribution coefficients in the two methods
- It is well-known that the relative error in the solution of the linear systems will depend on the condition number of the system matrix

#### **RECONSTRUCTION WITH SAMPLE MOMENTS**

$$\vec{c}_L = A\vec{m} \qquad \vec{c}_M = T^{-1}\vec{m}$$
$$\frac{\|\delta\vec{c}_L\|}{\|\vec{c}_L\|} \le \kappa (A) \frac{\|\delta\vec{m}\|}{\|\vec{m}\|} \qquad \frac{\|\delta\vec{c}_M\|}{\|\vec{c}_M\|} \le \kappa (T) \frac{\|\delta\vec{m}\|}{\|\vec{m}\|}$$
and due to the truncated SVD inversion of T:  $\kappa (T) \le \kappa (A)$ 

- Of course, the same SVD truncation could be performed on A too, but this extra effort renders the Legendre method somewhat slower than the moment method
- Hence, the moment method often is less sensitive to errors in the (sample) moments and it is faster
- Therefore, for many problems the moment method is preferred
- In some cases Legendre might still be preferable (for example multimodal and/or oscillatory distributions)

### POTENTIAL COEFFICIENTS AS A FUNCTION OF NUMBER OF PARTICLES



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#### FLUCTUATIONS IN LOW ORDER POTENTIAL COEFFICIENTS AS A FUNCTION OF INTEGRATION AND MOMENT ORDER



# COMPARISON OF THE POTENTIAL OF THE UNIFORM SQUARE, USING:

	Reconstructed distribution			
Analytical distribution	from truncated true	Reconstructed distribution		
		Trom sample moments- Thip		
I         COEFFICIENT         ORDER         EXPONENTS           1        3680282455232640         0         0         0         0         0           2         0.3926990816986540         2         2         0         0           3         0.208333333315265E-01         4         4         0         0           5        125000000010793         4         2         2         0           6         0.208333333315409E-01         4         0         4         0           7         0.5703792473055192E-12         6         6         0         0           9         0.1065048743642549E-01         6         2         0         0           9         0.1058513693363849E-10         6         2         0         0           10         0.5579089707580253E-12         6         0         0         1           1        3720238084313425E-03         8         0         0         0           14         0.1041666665699065E-01         8         2         0         0           15        3720238084185932E-11         10         10         0         0           16        1635264101592423E-11	I         COEFFICIENT         ORDER         EXPONENTS           1        3680282500557647         0         0         0         0           2         0.7436521970546914E-12         1         1         0         0           3         0.45551193291854E-11         2         1         1         0           4         0.3926990219829563         2         2         0         0           5         0.4653951393291854E-11         3         1         0         0           6         0.3926991414047079         2         0         2         0           7        1291820510685944E-10         3         2         0           9        1772742601284296E-10         3         1         0           10        9365479623203997E-11         3         0         0           11         0.208333828328526E-01         4         4         0         0           12        5782452636602210E-10         4         1         3         0           15         0.208333880688066E-01         4         0         4         1         3         0           16         0.1125494595861544E-09         5         5	I         COEFFICIENT         ORDER         EXPONENTS           1        3677357926229946         0         0         0         0         0           2        2858367532197177E-03         1         1         0         0         1         0         1           3        7350520101666331E-03         1         0         1         0         1         0           4         0.3922989592684850         2         2         0         0         1         0           5         0.1148352103807985E-03         2         1         1         0         0           6         0.3927646684209024         2         0         2         0         1           0        7679608989720461E-03         3         1         0         1         1         0         1           10        6312538437356915E-03         3         0         3         0         1         0           13        1253158193876644         4         2         2         0         1         1         0         1         0         15         0.1812030290642173E-02         5         0         0         1         0         14 <t< td=""></t<>		

# KICK MAP

- Once the Taylor expansion of the potential is computed, take derivative to obtain the fields in the beam frame
- Note that this is an elementary operation in DA, so there are no interpolation errors
- Lorentz boost to lab frame
- Substitute into the equations of motion
- Apply splitting and composition techniques
- Obtain space charge kick map from DA integration of the EOM in the same way as in the single-particle case

# **FLOW CHART**



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### MAP COMPARISON

#### Drift Map

1.000000	0.000000	0.000000	0.000000	0.000000	100000
1.000000	1.000000	0.000000	0.000000	0.000000	010000
0.000000	0.000000	1.000000	0.000000	0.000000	001000
0.000000	0.000000	1.000000	1.000000	0.000000	000100
0.5000000	0.000000	0.000000	0.000000	0.000000	030000
0.000000	0.000000	0.5000000	0.000000	0.000000	020100
0.5000000	0.000000	0.000000	0.000000	0.000000	010200
0.000000	0.000000	0.5000000	0.000000	0.000000	000300
0.3750000	0.000000	0.000000	0.000000	0.000000	050000
0.000000	0.000000	0.3750000	0.000000	0.000000	040100
0.7500000	0.000000	0.000000	0.000000	0.000000	030200
0.000000	0.000000	0.7500000	0.000000	0.000000	020300
0.3750000	0.000000	0.000000	0.000000	0.000000	010400
0.000000	0.000000	0.3750000	0.000000	0.000000	000500

#### Drift map with 1 space charge kick

-0.7852727E-05-0.1570545E-04 0.6368614E-07 0.1273723E-06	0.000000	000000
1.000616 0.1231262E-02-0.6734348E-05-0.1346870E-04	0.000000	100000
1.000000 1.000000 -0.1000220E-11 0.000000	0.000000	010000
-0.6734348E-05-0.1346870E-04 1.000612 0.1224478E-02	0.000000	001000
-0.1000220E-11 0.000000 1.000000 1.000000	0.000000	000100
-0.5143629E-04-0.1028726E-03-0.7751066E-05-0.1550213E-04	0.000000	200000
-0.2900714E-07 0.000000 0.1841803E-09 0.000000	0.000000	110000
-0.1177909E-04 0.000000 0.3184307E-07 0.000000	0.000000	020000
-0.1550213E-04-0.3100427E-04 0.1912624E-04 0.3825250E-04	0.000000	101000
0.3952803E-09 0.000000 -0.9616349E-08 0.000000	0.000000	011000
0.1841803E-09 0.000000 -0.9671336E-08 0.000000	0.000000	100100
0.6368614E-07 0.000000 -0.7852727E-05 0.000000	0.000000	010100
0.9563119E-05 0.1912625E-04 0.1205918E-05 0.2411835E-05	0.000000	002000
-0.9616349E-08 0.000000 0.3397128E-09 0.000000	0.000000	001100
-0.3926364E-05 0.000000 0.9552921E-07 0.000000	0.000000	000200

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### EXAMPLE

$$\frac{r_m}{r_0} = 1 + 5.87 \times 10^{-5} \frac{I}{(\gamma^2 - 1)^{\frac{3}{2}}} (\frac{z}{r_0})^{\frac{3}{2}}$$

Method	Growth
Edge Point x	35.27 %
Edge Point y	35.30 %
Map Element x	31.21 %
Map Element y	31.34 %





### **TUNE FITTING**



# SUMMARY

- Developed a theory of transfer maps for beams with space charge
- Numerical experiments show excellent results for some standard distributions
- It is general and flexible enough to be useful for a wide variety of beams and accelerators, both current and future
- Implementation into COSY is done
- Applications to date: UMER and MEIC
- <u>In summary</u>: as a consequence of the new methods we expect significant advances in space charge related phenomena understanding and mitigation in the near future