Analytical versus Numerical Integration in Satellite Geodesy

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„The purpose of computation is insight, not numbers“ (Hamming).

I Introduction and historical developments

In the near future a big step has again to be expected in satellite geodesy. Extremely precise measuring systems (accelerometer, low-low SST (relative accuracy 10^{-11}), gradiometer) in satellites orbiting as low as possible will allow not only the determination of the global gravity field in form of harmonic coefficients up to a limit somewhere below n = m = 180, but even the tracking of the extremely small signals in the gravity field due to mass redistributions in atmosphere, oceans and solid Earth down to the inner core.

An good understanding for all possible shortcomings in the data analysis process is required last but not least to avoid an interpretation of „geodetic observation errors“ as physical signals of mass redistributions.

Regarding the praxis of data analysis most professionals seem to be convinced today that only the use of numerical integration techniques will allow a reasonable analysis of these precise data.
We are now facing the danger that from two alternative and competitive procedures, namely

- the analysis in the time domain
- and the analysis in the spectral domain,

the latter will only insufficiently be supported. A meaningful analysis in the spectral domain, however, can only be performed on the basis of an analytical integration, since only an analytical solution connects the periodic effects in orbital data with the force parameters in a physically judicious mode.

The complete or general solution of N differential equations of first order contains a set of N arbitrary constants. Assigning particular numerical values to those constants one gets a so-called particular solution of the differential equation system.

Any numerical integration of an initial state problem corresponds to such a particular solution. By a suitable variation of the initial state vector (as well as the force parameters (variational equations)) one can generate a set of particular solutions.

From this set we usually pick up that particular solution which is in best agreement with observations, that is, which provides for the squares of the residuals the least sum (least squares adjustment).

However, a complete or general solution will be required for a clear and concrete understanding of the geometrical/physical nature of an energy process as well as for an understanding of the information at hand about this process, that are the gravity field parameters and the measurements. Those solutions are well-known in celestial mechanics and in satellite geodesy as analytical solutions; the derivation of such kind of solutions may be called analytical integration.

Perturbation theory is the general concept underlying both approaches, analytical and numerical integration. In the latter case a numerically derived orbit is used as a reference and afterwards the so-called variational equations are used to determine the „perturbations“ or corrections.

Analytical integration is more complex and based on several tools such as

- Problemoriented choice of orbital variables (Hill-, Kepler-, Delauney-variables, etc.)
- Infinitesimal transformation of variables based on series expansions (Trig. series, power series)

How did it come to the present situation, that is to an overestimation of the numerical integration approach and an underestimation of the analytical integration approach?

At the early times of satellite geodesy until the seventies only relatively inaccurate measurements (Baker-Nunn camera, Laser 1. generation) have been available. Based on analytical solutions (Brouwer, King-Hele, Kaula, Kozai, Gaposchkin etc.) special attention was devoted in particular to resonance effects, because only in relation to those effects the relatively inaccurate data could provide a reasonable signal/noise ratio. First developments of the so-called „lumped coefficient concept“, that is the analysis in the spectral domain, have later been carried on and extended, but only off the main path.

Due to the big jump in accuracy of the observations (Laser 3. generation, altimeter, GPS-phase observations) in the seventies the accuracy of the analytical solutions of first order (relative accuracy: 10^{-6}) as on hand at that time was insufficient for the analysis of those high precision data. We all have been forced at that time to restrict ourselves to numerical integration and analysis in the time domain; only this approach delivered the accuracy for the analysis of those high-precision data such as Laser and allowed the inclusion of all kind of force fields, gravitational and non-gravitational, in a systematic manner.

Of course, the praxis could not wait at that time whether eventually an analytical solution of high-precision would be developed under an inclusion of all kind of force fields in a systematic manner. As a result, the use of spectral analysis as a tool was very often considered with uneasy feelings and finally often not be clearly understood anymore.

A really alternative method of data analysis in the spectral domain could only be expected if an analytical solution could be developed of equally high accuracy as the numerical ones.

The authors have worked after a stay of the first author in the USA in 1975/76 to develop such kind of analytical solution. (Cui 1997) presents an analytical solution of second order (relative accuracy: 10^{-9}), which will be extended in the next future to a solution of third order (relative accuracy 10^{-12} corresponding to the accuracy of upcoming SST-data of 0.5×10^{-11}). An outline of the strategy for its further development is shown in (Cui 1999).

Some basic criteria which should guide the development of any analytical solution designed for data analysis in the spectral domain are given in the sequel.

Of course, at this stage we have to ponder and discuss again the merits and drawbacks of both approaches, the numerical and analytical one. The following article should be considered as a first attempt in this respect, probably still biased in the moment from the point of view of the authors.

II Some basic aspects of the numerical integration approach

A very good and pleasantly short description of the approach can be found in (Beutler 1996). However, to discuss merits and drawbacks some comments may be opportune which may be structured into 4 sections:

- Reference orbit and its differential equations
- Generation of reference orbit data (model data)
- Variation of parameters (state vectors and force parameters, auxiliary parameters)
- Spectral analysis of strings of data (orbital variables, model data, residuals, observations etc.)

Reference orbit. The 6 differential equations for an orbit (primary equations) can be numerically integrated using a suitable and sufficiently accurate technique if and only if **numerical values** are given for

- the parameters P_f of models for all force vectors $\mathbf{k}(P_f)$
- 6 (in case of SST 12) orbital variables $P_{isv}(t_0)$ describing position vector $\mathbf{r}(P_{isv})$ and velocity vector $\dot{\mathbf{r}}(P_{isv})$ at the reference epoch t_0 (initial state vector)

The movement of the center of mass of the satellite will further be described either by 6 instantaneous orbital variables $P_t(t)$ or by the 6 Cartesian components of the instantaneous state vectors $\mathbf{r}(t)$ and $\dot{\mathbf{r}}(t)$ at usually equidistant epochs $t = t_k$ (e.g. $t_{k+1} - t_k = 1\,\text{min}$); at any other epoch *t* the instantaneous state vectors may be obtained by a suitably chosen interpolation procedure.

In case an observation is connected to a station at the Earth surface (or to a point at the ocean surface as in altimetry), position and velocity of this station or point, respectively, must also be expressed by a function depending on time and certain constants, but we will restrict ourselves here to the simple case of SST.

The form of the differential equations will of course vary with the 6 orbital variables applied. The equations using Cartesian components as variables are given e.g. in (Beutler 1996). Using as an other example Hill variables we get the 6 differential equations

$$\begin{pmatrix} d\dot{r}/dt \\ dG/dt \\ dH/dt \\ dr/dt \\ du/dt \\ d\Omega/dt \end{pmatrix} = \begin{pmatrix} G^2/r^3 \\ 0 \\ 0 \\ \dot{r} \\ G/r^2 \\ 0 \end{pmatrix} + \begin{pmatrix} \partial V/\partial r \\ \partial V/\partial u \\ \partial V/\partial \Omega \\ 0 \\ -\partial V/\partial G \\ -\partial V/\partial H \end{pmatrix} + \begin{pmatrix} F_1 \\ rF_2 \\ r(\cos iF_2 - \sin iF_3) \\ 0 \\ (r/G)\cot i \sin uF_3 \\ r(G\sin i)^{-1}\sin uF_3 \end{pmatrix}$$

Here *V* is the gravity potential (geopotential, disturbing potential due to the other celestial bodies, tide induced potential, etc.) and F_i are the components of the non-gravitational forces with respect to the Gaussian basis (for details see Cui and Mareyen 1992).

Model data. Any data can be modeled as a function of the instantaneous orbital variables by including additional parameters P_m describing properties of the measurement process (e.g. eccentricity vector between center of mass and phase center of the antenna, tropospheric/ionospheric reduction model etc.):

$$\tilde{l} = \tilde{l}\left(\bar{X}_I(P_t), \bar{\dot{X}}_I(P_t), \bar{X}_{II}(P_t), \bar{\dot{X}}_{II}(P_t), P_m\right)$$

Those equations are called observation equations. Forming the differences with measured values *l*,

$$\Delta l = l - \tilde{l}$$

we get information how good our model describes the real process of motion.

Variation of parameters; Perturbations. We may look at the total differentials of the 6 instantaneous state variables as linear functions of the differentials of the initial state variables and the force parameters; that may be expressed by

$$[\Delta P_t] = \left[\frac{\partial P_t}{\partial P_{isv}}\right][dP_{isv}] + \left[\frac{\partial P_t}{\partial P_f}\right][dP_f].$$

The matrices of partial derivatives can be computed by the solution of a differential equation system, the variational equations.

The number of the equations of this system is equal to the number of the parameters P_{isv} (6 or 12, respectively) and P_f. If a huge set of force parameters should be determined from the data, as will be the case in SST, one is confronted with a huge variational equation system.

However, „whereas highest accuracy is required in the integration of the primary equations, the requirements are less stringent for the variational equations“ (Beutler 1996, p. 78). The equations

$$d\tilde{l} = \left[\frac{\partial \tilde{l}}{\partial P_t}\right][dP_t] + \left[\frac{\partial \tilde{l}}{\partial P_m}\right][dP_m]$$

are called linearized observation equations (sometimes misleading also variational equations) in case the parameters $P = \{P_{isv}, P_f, P_m\}$ are considered as unknowns in an adjustment procedure.

Spectral analysis and mean orbit. This is by far the weakest point in the pure numerical integration approach. Of course, one can always use an empirical spectral model; the orbit length (short/long arc) provides then the smallest and the numerical integration step the highest frequency.

However, those empirical frequencies depend on an arbitrary chosen computation model and have nothing to do with the frequencies of the orbit perturbations generated by the physical forces. In fact, people often skip the spectral investigations therefore, presenting as a substitute illustrating pictures (see e.g. Beutler 1996, p. 59ff).

Since „the osculating elements are not well suited to study the long term evolution of the satellite systems“ so-called mean elements are often introduced. „The purpose is the same in all cases: one would like to remove the higher frequency part of the spectrum in the time series of the elements“.

„There are many different ways to define mean orbital elements starting from a series of osculation elements.“ In fact, there is, but only if an arbitrarily defined empirical spectrum is introduced and certainly **not** if the generating forces will define the spectrum as it corresponds to reality.

III Some basic aspects of the analytical integration approach

Regarding satellite data analysis one can hardly overestimate one big advantage of analytical orbit integration: spectral analysis or the „lumped coefficient concept“, respectively, may not only be used for efficient algorithms but over all for a much better insight into the information content of data.
Having this in mind an efficient analytical solution should be designed fulfilling some important criteria, among them at least

1) The global accuracy of analytical integration should meet all present and future accuracy requirements
2) A suitable technique for comparisons with results of numerical integration should be available
3) It must be possible to introduce all kind of force fields in a systematic and unified manner
4) The analytical solution should be designed to be as efficient as possible for applications of spectral analysis techniques
5) Regarding applications the basic structure of the analytical solution should be most simple and lucid even though details may remain fairly complex.

Those criteria have been developed in the course of the derivation of a second order solution which will be used here to illustrate those general comments in this section.

1) The global (and not just some local) accuracy of analytical solutions can be determined in powers of $\varepsilon = c_{2(0)} \approx 10^{-3}$. We have to distinguish

- solutions of first order: $\varepsilon^2 \approx 10^{-6}$ (e.g. Kaula’s solution)
- solutions of second order: $\varepsilon^3 \approx 10^{-9}$ (e.g. Cui’s solution)
- solutions of third order: $\varepsilon^4 \approx 10^{-12}$ (in development)

The accuracy requirements depend of course strongly on the data accuracy. Upcoming SST-data of the GRACE-mission will have a relative accuracy of 0.5×10^{-11}; therefore a third order solution would be necessary if numerical integration should entirely be avoided in the data analysis process. For the solution of the variational equations a second order solution only will be sufficient.

2) In view of a comparison of numerical and analytical integration one has to recognize the fact that the technique of numerical integration is extremely inflexible in contrast to analytical ones. As a consequence the analytical solution must be adopted to the numerical ones.

Principally, the analytical solutions are based on the parameters of a mean orbit, the numerical ones on the numerical values for the orbital variables describing the initial state vector.

The inverse analytical solution, that is, the computation of the elements of the mean orbit from given initial (or any instantaneous) state vector is of utmost importance in view of comparisons with numerical integration results.

Moreover, the inverse analytical solution will provide a very efficient tool for the definition of a physically meaningful mean orbit.

Last but not least the inverse analytical solution will provide an extremely efficient tool to use also in satellite data analysis the traditional geodetic concept of data reduction with the goal to simplify the functional model. As well-known this concept is very often and efficiently applied in other domains of geodesy, where it has a long tradition.

A technique to proceed from the initial state vector to elements of the mean orbit and vice versa is described in (Cui and Lelgemann 1995).

3) Regarding the force field it is of uppermost importance that physically two completely different sources of forces govern the orbit

- gravitational forces (Earth and Earth-tide, Moon, Sun etc.),
- non-gravitational or surface forces (air drag, radiation pressure etc.).

The instantaneous state variables may be separated into the sum

$$P_t(t) = \overline{P}_t(t) + \delta P_{fg}(t) + +\delta P_{fs}(t)$$

The perturbations of the orbital variables due to non-gravitational forces are always defined as being zero at the initial state epoch t_0. Those orbit perturbations are growing irregularly; their description using trig. functions may therefore not an efficient concept.

The best way to proceed may be the following. The instantaneous surface force can be expressed by its components with respect to the Gaussian basis in form of an empirical time series (numerical values at equidistant ($\Delta t = const$) epochs

- either using data of an accelerometer as foreseen for the GRACE-mission
- or otherwise using an empirical model such as developed in (Arfa-Karboodvand, 1997)

Using the observation equations for the Hill variables (see section 1) together with crude and approximate instantaneous orbital variables one can express the effect of the surface forces accurate enough by empirical, equidistant epoch data $F_i^{sf}(t_k)$.

4) It can be shown that furthermore **all** gravitational forces will result in a **secular** movement just only of the ascending node (right ascension of the ascending node Ω) and of the perigee (argument of perigee ω) of a quasi-secular rotating ellipse as a reference (mean) orbit. All gravitational induced perturbations of such a reference orbit are then purely periodic (inclusive constant terms), having the simple functional form

$$\delta P_t = \sum_q \sum_m \sum_k \left[a_{kmq}(i, G, e; P_{fg}) \cos(ku + mh + qf) + b_{kmq}(i, G, e; P_{fg}) \sin(ku + mh + qf) \right]$$

where u, $h = \Omega - \Theta$ and f are the argument of latitude, the geographical longitude of ascending node and the true anomaly, all of the reference orbit.

The amplitudes of the trig. functions depend on the constant orbital elements i, G and e of the reference orbit as well as on the gravitational force field parameters. They are often called „lumped coefficients“ in the literature.

We have already checked that a third order solution will have the same structure, that is, very small additional terms only for the periodic perturbations have to be added to a second order solution (Cui 1999).

Theoretically, the summations have to be extended to the limits $-\infty < k < \infty$, $0 \le m < \infty$ and $-\infty < q < \infty$, but for applications the smallest summation limits should be fixed according to the accuracy requirements.

Despite some details of the solution may be fairly complex (see e.g. Cui 1997) its basic structure is obviously very simple.

The solution can also approximately be expressed by reducing the numbers of angular variables.

In case of nearly circular orbits it can be shown that the true anomaly can be expressed with sufficient accuracy as a function of the argument of latitude

$$f = (1-\sigma)u + const$$

where $\sigma = \sigma\left(i, G; \tilde{P}_{fg}\right) = O\left(c_{2(0)}\right)$ is a very small number and $\tilde{P}_{fg}$ is a subset of the gravitational force field parameters.

In case of geosynchronous (repeating) orbits there will be a fixed ratio between the revolutions of the satellite and of the Earth,

$$-\frac{\dot{u}}{\dot{h}} = \frac{\dot{u}}{\dot{\Theta} - \dot{\Omega}} = \frac{p}{q}, \qquad p, q = \text{integer numbers}$$

that is, during q revolutions of the Earth the satellite will perform p revolutions. In such cases the perturbations can be expressed as a function of just one angular variable.

In case of so-called „deep resonance“ (critical inclination $i = 63.4°$, exact polar orbits $i = 90°$, geosynchronous orbits) some lumped coefficients will become infinitely large whereas the corresponding frequency becomes infinitely small. With other words the perturbations become similar to secular effects. In this case a Taylor series expansion may be used together with Encke’s technique. The same method may also be used to investigate possible coupling effects of gravitational with non-gravitational forces.

5) Regarding the application of analytical solutions for spectral analysis we may separate the (linearised) observation equation system into

$$\left[d\tilde{l}\right] = \left[\frac{\partial \tilde{l}}{\partial P_{isv}}\right]\left[dP_{isv}\right] + \left[\frac{\partial \tilde{l}}{\partial P_{fg}}\right]\left[dP_{fg}\right] + \left[\frac{\partial \tilde{l}}{\partial P_{fs}}\right]\left[dP_{fs}\right] + \left[\frac{\partial \tilde{l}}{\partial P_{m}}\right]\left[dP_{m}\right]$$

that is, into terms according to

- initial state variables P_{isv} (or mean orbit variables $\overline{P}$)
- gravity force field parameters P_{fg}
- surface force parameters P_{fs}
- measurement technique related parameters P_m

If as a goal the determination of the gravity field is intended the second term will be of major importance. Neglecting just for the moment the two last terms we may express even the **non-linear** observation equations in the form

$$\tilde{l} = \tilde{l}_0\left(\overline{P}\right) + \delta\tilde{l}$$

where $\delta\tilde{l}$ may be expressed by a formula similar to those for the perturbations of the orbital variables (see Cui 1997)

$$\delta\tilde{l} = \sum_q \sum_m \sum_k \left[a_{kmq}\left(i, G, e; P_{fg}\right)\cos\left(ku + mh + qf\right) + b_{kmq}\left(i, G, e; P_{fg}\right)\sin\left(ku + mh + qf\right)\right],$$

where a_{kmq} and b_{kmq} are now the lumped coefficients of the observable *l*.
Consequently, we may separate the corresponding matrix into the product of two matrices

$$\left[\frac{\partial\tilde{l}}{\partial P_{fg}}\right] = \left[\frac{\partial\tilde{l}}{\partial a_{kmq}} \;\middle|\; \frac{\partial\tilde{l}}{\partial b_{kmq}}\right]\begin{bmatrix}\dfrac{\partial a_{kmq}}{\partial P_{fg}} \\ \dfrac{\partial b_{kmq}}{\partial P_{fg}}\end{bmatrix} = \mathbf{BT}$$

This separation is fundamental for the application of the „lumped coefficient concept“, that is the spectral analysis technique.

The matrix $\mathbf{N} = \mathbf{B}^T\mathbf{B}$ will become for a sufficient length of a data set a **diagonal dominant** matrix, in the case of an unlimited length of the data set a diagonal one.

The matrix **T** is a **very sparse** matrix separating into small diagonal block matrices connecting the gravity force field parameters P_{fg}, among them in particular the harmonic coefficients c_{nm} and s_{nm}, with the lumped coefficients.

The effects of a variation of either the mean variables or the initial state variables must be carefully analyzed with respect to the question whether periodic effects will occur with analogue frequencies as due to gravitational force effects in order to avoid aliasing in the framework of a determination of force parameters P_{fg}.

The same must be done for effects of a variation of surface forces or of auxiliary parameters P_m on the data. If aliasing may occur the determination of the force parameters must be done with extreme due care.

The spectral analysis technique was already extremely helpful in the framework of altimeter data analysis. Using older GEOSAT-ephemeris provided by NOAA with a radial orbit error of about 5 m it turned out that the largest part of those orbital errors have been generated by the use of an inadequate Earth gravity model; the radial orbital error could be reduced to 0.30 m using crossover-differences as data (Cui and Lelgemann 1995). In contrast, as a study in progress has shown, the orbital error of ERS-ephemeris of about 10 cm **cannot** be explained by an insufficient Earth gravity field model.

In any case such kind of investigations can only be done in the spectral domain on the basis of a precise and suitably designed analytical solution.

IV Numerical versus analytical integration

Having in mind a comparison of the results of both approaches we have to clarify first for an unbiased judgement possible problematic sides of both techniques, since those may be the origin of imperfections of the results.

Since the authors had uneasy feelings with a pure numerical approach they have started two decades ago with the development of a precise analytical solution of higher order. Those uneasy feelings are based on the following arguments.

1) Insufficient cognition of the information content of a specific kind of observational data (like Laser, altimeter, SST etc.), that is, insufficient cognition of the unknowns which can unobjectively be determined from those observations.
2) Insufficient comprehension of the „correlation“ effects occurring in the determination of the unknowns in case of a completely filled up (not-sparse), bad conditioned normal equation matrix of huge size (more than 30,000 unknowns in case of a gravity field resolution of $n=m<180$). The computation of the correlation matrix will never be sufficient for a necessary insight.
3) Extremely high may be the also danger that near the absolute minima for the sum of pvv there are relative minima. In such a case it depends just on the approximate starting values for the unknowns in the Newton-Raphson iteration which minima will be reached with the final solution.
4) Insufficient knowledge about the effects of the definition of the orbital arc length (short arc, long arc). An unobjectionable determination of the force parameters will only be possible if aliasing of force effects into the initial state parameters is excluded.
5) Insufficient knowledge about the frequencies of a given data string, that is, about the forms in the variation of measurements generated by specific force field components, by a variation of initial state parameters etc.
6) Insufficient knowledge about the consequences of deep resonance effects which occur for geosynchronous orbits (repeating orbits) as often chosen for Earth observing or navigational satellites.

Moreover, the error estimate of analytical integration (e.g. 10^{-12} for a theory of 3. order) is always a global error estimate. In contrast, numerical integration provides in fact efficient local error estimates, but poorly global ones.

7) Insufficient **global** error estimates in case of very low flying satellites (large longperiodic superimposed by very small shortperiodic disturbations), that is, if very small step sizes are required.
8) Error estimation in case of huge systems of more than 30,000 variational equations as will occur in SST-data analysis.

All those possible problems must be carefully considered in case of e.g. SST-data analysis. For the case of analytical integration approaches the authors do not see similar problems, but of course our point of view may be biased and an „advocatus diabolus“ would be desirable.

One problem using analytical integration may be the correctness of the complex formulas connecting the lumped coefficients with the force parameters. Good theoreticians may check, however, the derivation of those formulas on the one hand and comparisons with simulation results using numerical integration may give hints about yet incorrect analytical terms.

Despite the fact that a lot of individual objectives remain to be investigated the basic concepts for at least one high-precision analytical solution (there may be other analytical methods providing an even more efficient or a simpler solution) has been developed providing an alternative method to the numerical integration approach for the analysis of the extremely precise tracking data as will come up in the near future.

V Final remarks

This article was not written to stir up war between partisans of the analytical and the numerical approach. But it is a fact that we have two alternative concepts to analyze the SST-data obtained in the next future from expensive missions and **we should use both concepts**.

The basic theoretical developments for spectral domain analysis have already been performed and the next steps (e.g. software developments, simulation studies, analysis of measurements) will require team work and with this financial support. The development of todays high-precision numerical approach software was very time consuming and expensive; the future development in the framework of a high-precision analytical approach will certainly be faster and cheaper.

It seems to be urgent now to discuss openly possible merits and shortcomings of both approaches and over all use both methods or moreover a combination of both, a semi-analytical one, for the data analysis.

The comparison of the results of both techniques may startle both sides but will certainly give, according to our opinion, an enormous progress not only for the theoretical foundation of our beloved science but also for the interpretation of the results of the new geodetic satellite missions.

Acknowledgment

Dear Erik. „**Nichts ist so praktisch wie eine gute Theorie**“ has, like all good proverbs, two meanings. It provides not only a definition for the conception „good theory“ but states also how important theory may be for practical work. You have always insisted that the theoretical background of geodesy has to be cleared and extended in our times of fast progressing observation techniques and computers. Thank you for this insistence, old buddy.

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