Works by Guri Marchuk on numerical mathematics and its applications

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1953–1962: G.Marchuk developed the integral-interpolation method and theory of difference schemes for nuclear reactor problems.

He suggested an effective way to replace the original differential problem by the system of integral identities.

Marchuk's integral identity

Applied to the equation

$$-\frac{1}{x^\alpha}\frac{d}{dx}\left(x^\alpha p(x)\frac{d}{dx}\varphi(x)\right) + q(x)\varphi(x) = f(x), \quad x \in (a,b),\ 0 \le \alpha < 1,$$

with $p(x) > 0, q(x) \ge 0, f(x)$, the identity has the form

$$\frac{\varphi(x_k) - \varphi(x_{k+1})}{[1/p]_{k+1/2}} + \frac{\varphi(x_k) - \varphi(x_{k-1})}{[1/p]_{k-1/2}} + \int\limits_{x_{k-1/2}}^{x_{k+1/2}} \Phi(x)dx =$$

$$= -\left[\frac{1}{p}\right]_{k+1/2}^{-1}\left[\frac{1}{p}\int\limits_{x_{k+1/2}}^{x}\Phi(t)dt\right]_{k+1/2} + \left[\frac{1}{p}\right]_{k-1/2}^{-1}\left[\frac{1}{p}\int\limits_{x_{k-1/2}}^{x}\Phi(t)dt\right]_{k-1/2},$$

where

$$\Phi(x) = x^\alpha(q(x)\varphi(x) - f(x)),\ [\psi]_{k\pm1/2} = \int\limits_{x_{k-1/2\pm1/2}}^{x_{k+1/2\pm1/2}} \psi(x)dx/x^\alpha.$$

Numerical schemes of 1970-80s

The 1970-80s: G.Marchuk and his disciples developed the thery of difference and variational-difference schemes for various problems of mathematical physics (kinetic equations, elliptic, parabolic, and hyperbolic problems).

G.Marchuk and V.Agoshkov. Introduction to Projective-Difference Methods (1981):

Effective projective-difference algorithms were developed, based on special choice of basis functions taking into account the specifics of solutions of the original problem.

G.Marchuk and V.Shaidurov. Improving the Accuracy of Solutions of Difference Schemes (1980):

Use of the grid sequences for improving the accuracy of solutions of difference schemes (multigrid). Development of the Richardson extrapolation method for many classes of problems (ODE, PDE, time-dependent problems etc.) The original extrapolation method of the small parameter, accounting the specific behavior of the solution.

G.Marchuk. Methods of Numerical Mathematics (1980):

Methods and theory of difference schemes.

Splitting methods

Method of splitting with respect to physical processes: reduction of the original problem to a sequence of simple problems governing elementary physical processes. Absolutely stable difference schemes of the second-order approximation for solving nonstationary problems of mathematical physics and geophysics.

Marchuk's two-cyclic splitting method

For the evolution equation

$$\frac{d\varphi}{dt} + A\varphi = f, \quad A = \sum_{i=1}^{n} A_i(t), \; A_i(t) \geq 0,$$

G.Marchuk suggested two-cyclic splitting:

$$\left(E + \frac{\tau}{2}A_1^j\right)\varphi^{j-(n-1)/n} = \left(E - \frac{\tau}{2}A_1^j\right)\varphi^{j-1},$$

$$\dots$$

$$\left(E + \frac{\tau}{2}A_n^j\right)(\varphi^j - \tau f^j) = \left(E - \frac{\tau}{2}A_n^j\right)\varphi^{j-1/n},$$

$$\left(E + \frac{\tau}{2}A_n^j\right)\varphi^{j+1/n} = \left(E - \frac{\tau}{2}A_n^j\right)(\varphi^j + \tau f^j),$$

$$\dots$$

$$\left(E + \frac{\tau}{2}A_1^j\right)\varphi^{j+1} = \left(E - \frac{\tau}{2}A_1^j\right)\varphi^{j+(n-1)/n},$$

where $A_i^j \geq 0$, with approximation τ^2, and absolutely stable.

Splitting method developments

G.Marchuk and N.Yanenko, IFIP Congress (1965): Splitting methods for intergo-differential equtions.

G.Marchuk and V.Kuzin: Development of algorithms to construct appoximations of $\{A_i^j\} \geq 0$, using special grids in finite element methods.

G.Marchuk and U.Sultangazin, G.Marchuk and V.Penenko: Development of splitting methods for transport theory problems.

G.I.Marchuk. Splitting Methods (1988).

G.I. Marchuk. Splitting and Alternating Direction Methods. Handbook of Numerical Analysis (1990) (P.G. Ciarlet. J.L. Lions, eds.), North-Holland.

Adjoint equations

G.Marchuk, V.Orlov. To the thery of adjoint functions (1961): method to construct adjoint functions φ_p^* (value functions) for a wide class of linear problems:

$$A\varphi = f.$$

For the functional

$$J_p(\varphi) = (\varphi, p),$$

where p is related to a physical process, the adjoint function φ_p^* was introduced as a solution to the adjoint equation

$$A^*\varphi_p^* = p,$$

with the right-hand side p from the functional $J_p(\varphi)$. This leads to a dual representation of the functional:

$$J_p(\varphi) = (\varphi_p^*, f).$$

Perturbation theory

With the use of adjoint functions, the formulas of perturbation theory were derived for corrections of functionals when instead of the operator A the perturbed operator $A' = A + \delta A$ was considered.

In particular, the first-order perturbation formulas

$$\delta J_p = -(\varphi_p^*, \delta A \varphi) = -(\varphi, \delta A^* \varphi_p^*),$$

were widely applied for estimation of various effects in complex systems.

Statement of inverse problems

Using the adjoint equations and perturbation theory, G.Marchuk (1961) suggested a general statement of inverse problems to restore the parameters or functions $\{\alpha_k\}$, $\{\beta_k\}$ in the operator

$$A = \sum_{k=1}^{m} \Big(\alpha_k A_k + B_k(\beta_k C_k) \Big)$$

(where A_k, B_k, C_k - some linear operators), given a set of functionals (measurements) J_{p_i}, $i = 1, \ldots, n$. With the use of small perturbation formulas, the system was derived

$$\sum_{k=1}^{m} \Big[(\varphi^*_{p_i}, \delta\alpha_k A_k \varphi) + (B^*_k \varphi^*_{p_i}, \delta\beta_k C_k \varphi) \Big] = \delta J_{p_i},$$

where the adjoint function $\varphi^*_{p_i}$ is the solution of $A^* \varphi^*_{p_i} = p_i$, and φ is the solution to the original problem $A\varphi = f$. The algorithms were developed to find the corrections $\{\delta\alpha_k\}, \{\delta\beta_k\}$. As a result, the inverse problem was reduced to a problem of linear algebra.

Monte Carlo

G.Marchuk. Equation for value of information from meteorological satellites and statement of inverse problems (1964): General statement of inverse problems applied to atmospheric optics.

G.Marchuk, G. Mikhailov et al. Monte Carlo Method in Atmospheric Optics (1976): Statistical methods for solving inverse problems.

G.Marchuk, G. Mikhailov et al. USSR State Prize (1979): Development and application of methods for statistical modelling.

Adjoint equations for nonlinear problems

G.Marchuk (1974) introduced adjoint to a quasilinear operator $A(\varphi)$ by

$$(A(\varphi), \psi) = (\varphi, A^*(\varphi)\psi),$$

where $A^*(\varphi)$ is linear with respect to ψ and depends on the solution φ of the original (direct) problem $A(\varphi) = f$. The adjoint function φ_p^* (*value function*) was defined as the solution of the adjoint equation $A^*(\varphi)\varphi_p^* = p$.

G.Marchuk, V.Agoshkov (1986): new principle of constructing the adjoint operators for a wide class of nonlinear problems, based on the Newton-Lagrange formula.

G.Marchuk, V.Vladimirov (2000): Adjoint operator in nonlinear case was derived from an equivalence class of linear operators.

G.Marchuk. Adjoint Equations (1992), Nauka.

G.Marchuk. Adjoint Equations and Analysis of Complex Systems (1995).

G.Marchuk, V.Agoshkov, V.Shutyaev. Adjoint Equations and Perturbation Algorithms in Nonlinear Problems (1996), CRC Press.

G.Marchuk (1950s): Application of matrix factorization methods for solving the systems of algebraic equations, development of iterative methods to compute minimal eigenvalues of multidimensional difference operators.
G.Marchuk (1960s): New variational principle of construction and optimization of iterative methods. For a system in the general form

$$Au = f$$

the iterative methods are given by the formula

$$u^k = u^{k-s} - \sum_{i=1}^{s} \alpha_{k,\,i} B_i (Au^{k-i} - f),$$

where B_i are some matrices, and the parameters $\alpha_{k,\,i}$ are chosen by the global minimization of a given quadratic functional (e.g. generalized CGs.)

G.Marchuk, Yu.Kuznetsov. Iterative Methods and Quadratic Functionals (1972): Theory of iterative methods. Fictitious component method.

Methods for nuclear reactors

G.Marchuk. Numerical methods for nuclear reactor calculations (1958)

G.Marchuk. Methods for nuclear reactor calculations (1961).

G.Marchuk solved the problem of correct transition from the Boltzmann equation

$$(\Omega, \nabla)\varphi + \sigma\varphi = \int dv' \int W(x, \mu_0, v' \to v)\varphi(x, \Omega', v')\, d\Omega'$$

to effective few-group models of the form

$$(\Omega, \nabla)\varphi^j + \sigma^j\varphi^j = \sum_l \int W^{l\to j}(x, \mu_0)\varphi^l(x, \Omega')\, d\Omega',$$

where $\sigma^j, W^{l\to j}$ are the group constants.

Adjoint equations for group constants

G.Marchuk developed the methods for constructing the group constants. The formulas for σ^j, $W^{l\to j}$ were derived:

$$\sigma^j = \int_{G_n} dx \int \varphi^{*j}\, d\Omega \int_{v_{j-1}}^{v_j} \sigma\varphi\, dv \Big/ \int_{G_n} dx \int \varphi^{*j}\, d\Omega \int_{v_{j-1}}^{v_j} \varphi\, dv,$$

$$W^{l\to j}(x,\mu_0) = \Delta v_j \sum_{m=0}^{\infty} \frac{2m+1}{2} W_m^{l\to j} P_m(\mu_0),$$

where

$$W_m^{l\to j} = \frac{\displaystyle\int_{G_n} \varphi_m^{*j}\, dx \int_{v_{l-1}}^{v_l} \varphi_m\, dv \int_{v_{j-1}}^{v_j} W_m(x, v\to v')dv'}{\displaystyle\int_{G_n} \varphi_m^{*j}\, dx \int_{v_{l-1}}^{v_l} \varphi_m\, dv}.$$

Nuclear reactor calculations

Physics and Power Engineering Institute (Obninsk): one of the first USSR software was developed for nuclear reactor calculations, based on the methods developed by G.Marchuk and his colleagues. E.g., it was used for serial calculations of critical masses, for the first nuclear power plant.

G.Marchuk et al. USSR Lenin Prize (1961): calculations of nuclear reactors for submarines.

G.Marchuk and V.Smelov: Spherical harmonics method, matrix factorization.

G.Marchuk and V.Lebedev. Numerical methods in neutron transport theory (1971, 1981): Theory of numerical methods for neutron transport problems.

Variational data assimilation

DA problem: find u and φ such that

$$\begin{cases} \dfrac{\partial \varphi}{\partial t} & = & F(\varphi) + f, \quad t \in (0, T) \\ \varphi\Big|_{t=0} & = & u, \\ J(u) & = & \inf\limits_{v \in X} J(v), \end{cases}$$

where

$$J(u) = \frac{1}{2}(V_b^{-1}(u - u_b), u - u_b)_X + \frac{1}{2}(V_o^{-1}(C\varphi - y), C\varphi - y)_{Y_o}$$

with the background function $u_b \in X$, the observations $y \in Y_o$, $C : Y \to Y_o$ being an observation operator, and Y_o an observation space.

G.Marchuk (1961), V.Penenko (1975), G.Marchuk and V.Penenko (1977), F.-X. Le Dimet (1982).

Optimality system

The necessary optimality condition reduces the DA problem to the following system:

$$\begin{cases} \dfrac{\partial \varphi}{\partial t} & = & F(\varphi) + f, \quad t \in (0, T) \\ \varphi\big|_{t=0} & = & u, \end{cases}$$

$$\begin{cases} -\dfrac{\partial \varphi^*}{\partial t} - (F'(\varphi))^* \varphi^* & = & -C^* V_o^{-1}(C\varphi - y), \quad t \in (0, T) \\ \varphi^*\big|_{t=T} & = & 0, \end{cases}$$

$$V_b^{-1}(u - u_b) - \varphi^*\big|_{t=0} = 0$$

with the unknowns φ, φ^*, u, where $(F'(\varphi))^*$ is the adjoint to the Frechet derivative of F, and C^* is the adjoint to C defined by $(C\varphi, \psi)_{Y_o} = (\varphi, C^*\psi)_Y$, $\varphi \in Y, \psi \in Y_o$.

Iterative algorithms for DA

A class of iterative algorithms for solving the optimality system:

$$\frac{d\varphi^k}{dt} + A(t)\varphi^k = f,\ t \in (0, T); \quad \varphi^k(0) = u^k,$$

$$-\frac{d\varphi^{*k}}{dt} + A^*(t)\varphi^{*k} = C(\hat{\varphi} - \varphi^k),\ t \in (0, T); \quad \varphi^{*k}(T) = 0,$$

$$u^{k+1} = u^k - \alpha_{k+1} B_k(\alpha(u^k - \hat{\varphi}^\circ) - \varphi^{*k}\big|_{t=0}) + \beta_{k+1} C_k(u^k - u^{k-1}),$$

where B_k, C_k are some operators, α_{k+1}, β_{k+1} are iterative parameters.

G.Marchuk and V.Agoshkov (1993), G.Marchuk and V.Zalesny (1993), G.Marchuk and V.Shutyaev (1994).

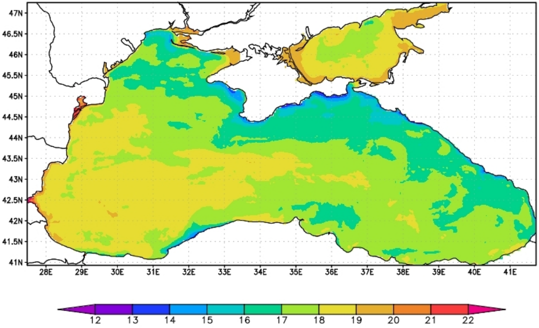
G.Marchuk. Adjoint Equations and Analysis of Complex Systems (1995).

G.Marchuk, V.Agoshkov, V.Shutyaev. Adjoint Equations and Perturbation Algorithms in Nonlinear Problems (1996), CRC Press.

Projects for DA

The Information Data Processing System (2012) of variational assimilation was developed at INM RAS in application to the Black Sea model.

2011-2013: Joint project of Russian Academy of Sciences and National Academy of Sciences of Ukraine, "The Black Sea as an imitation model of the ocean"(leaders - academician G. Marchuk and academician B.Paton): Further development of methods for data assimilation in ocean models.



Selected Works of G.I.Marchuk

Volume 1: Methods of Numerical Mathematics
(Resp. Editor V.Agoshkov)

Volume 2: Adjoint Equations and Analysis of Complex Systems
(Resp. Editor V.Zalesny)

Volume 5:
Numerical Methods for Nuclear Reactor Calculations
(Resp. Editor V.Shutyaev)

Thank you!