St Petersburg University
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Joint Institute for Nuclear Research
Meshcheryakov Laboratory of Information Technologies
10
GRID2023
3-7 July 2023
10th International Conference
"Distributed Computing and Grid Technologies in Science and Education"

Mathematics as an engine for computational sciences

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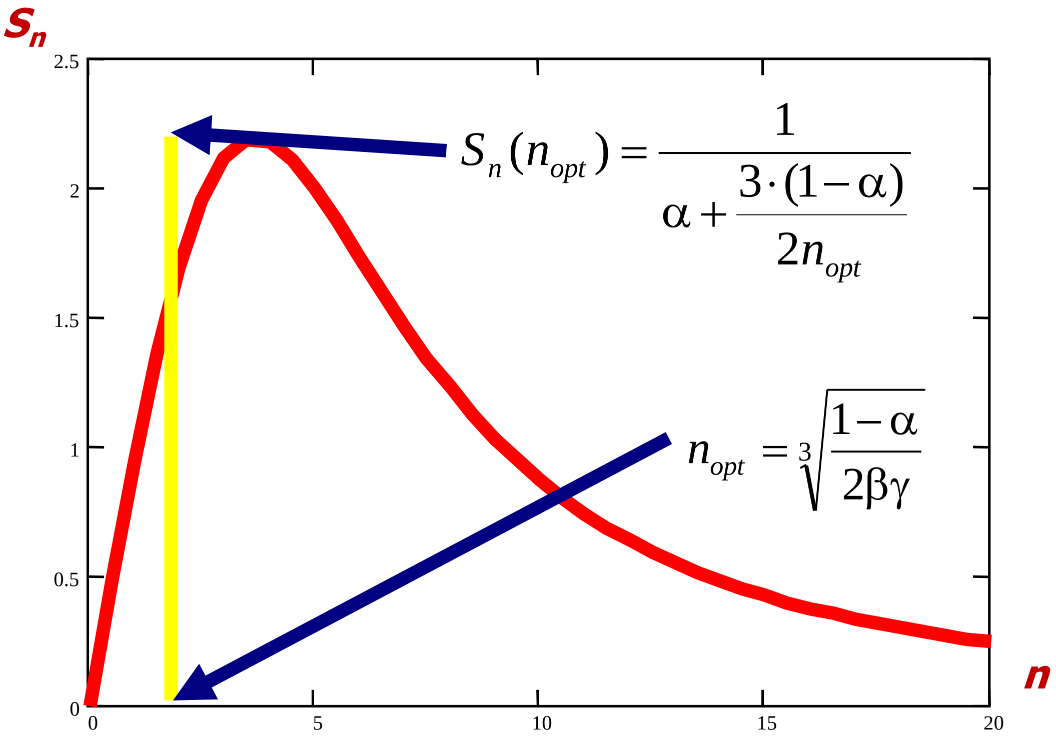
What we need to understand

1. The problems of classical architectures
2. Hopes with quantum systems
3. Why quantum computing anyway
4. What about underlying mathematics
5. How to improve it
6. Can we use quantum math in practice
7. Parallel algorithms
8. A way to qualitative analysis

Typical shape of cluster acceleration

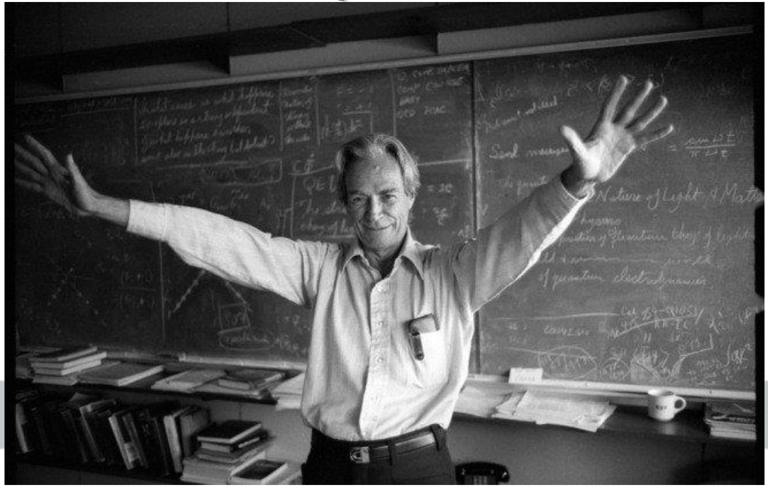


Quantum supremacy

The concept of a qualitative quantum computational advantage, specifically for simulating quantum systems:

“Nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem, because it doesn't look so easy.”

R. Feynman



Church–Turing thesis

Any computational problem that can be solved by a classical computer can also be solved by a quantum computer. Conversely, any problem that can be solved by a quantum computer can also be solved by a classical computer, at least in principle given enough time

Problems: bits and qubits,

need of measurement,

stability of quantum system,

quantum analog systems

While we wait for quantum computer,

Let us turn to quantum computing

R. Feynman prophesy the need of new math for quantum computing and claimed path integral to be the tool

$$G(X, X') = \int DX\ exp\{i/hS_d(X, X')\}$$

$$DX = \Pi_t A dx, \qquad A = (2\pi i h\gamma)^{-1/2}$$

The limit does't exist

Feynman idea: to use

$$(2\pi i h\gamma)^{-1/2} = \int dp\, exp(i/h\gamma[p - \{x' - x\}]^2)$$

to get

$$G(X, P) = \int DP\, D\, X/(2\pi h)^s\, exp\left\{i/h \int XdP - i/h \int Hd\alpha + i\phi\right\}$$

with $DP\, DX = \Pi_t dp\, dx$

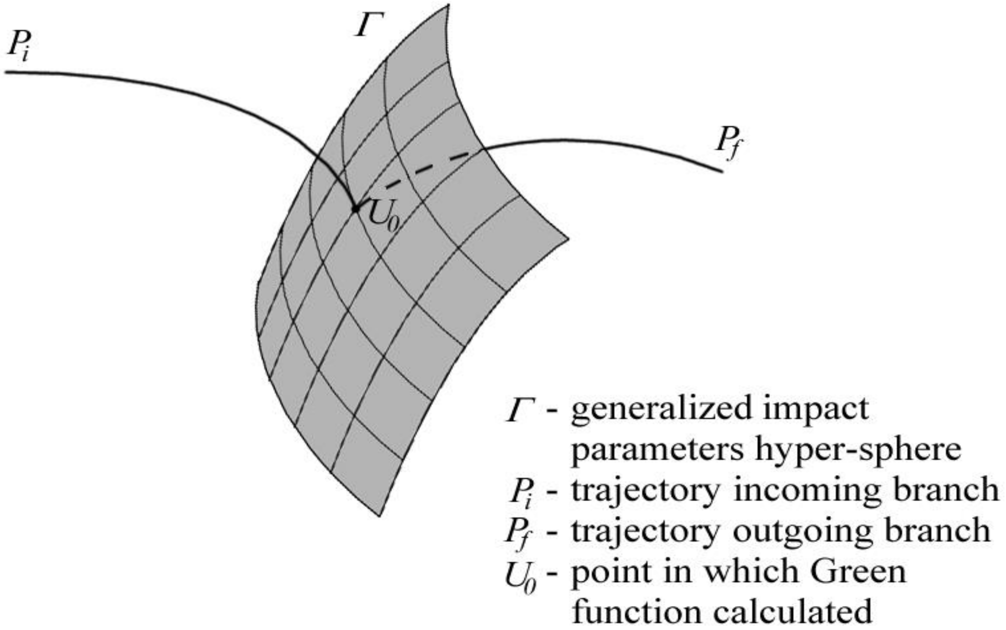
The problem: in finite presentation number of integrations over p and x is different

How to solve

1. If ends are coordinates insert one more integral with delta function and make a shift of coordinate by t p (V. Popov, L. Faddeev)

2. If ends are momentums take one internal integral, represent next momentum over previous and again make shift (A. Bogdanov et al.)

The result is

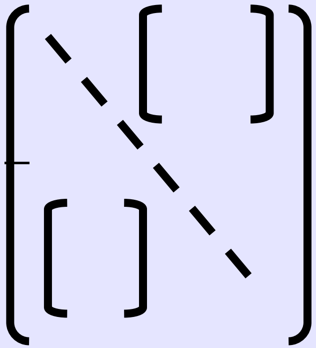


$$A(i, f') = \langle G(i,t) G(t, f') \rangle$$

The difference with standard approach

$$i\hbar \partial\Psi/\partial t = H\Psi \Rightarrow$$

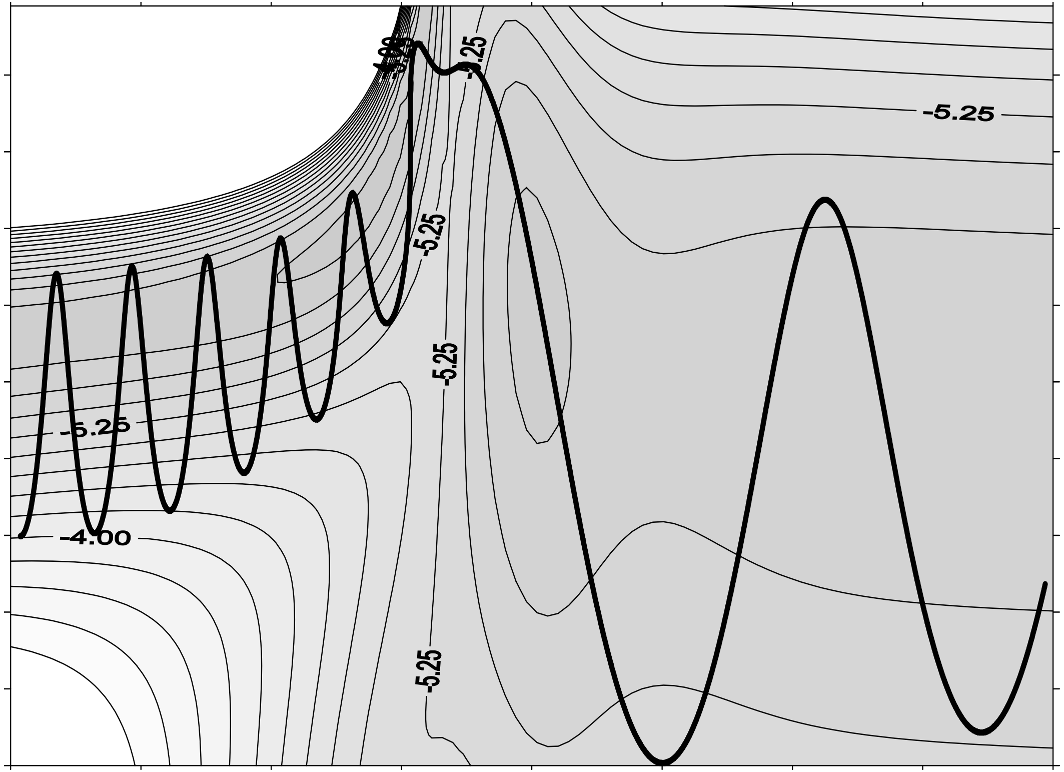
$$i\partial a/\partial t = Aa \quad A =$$



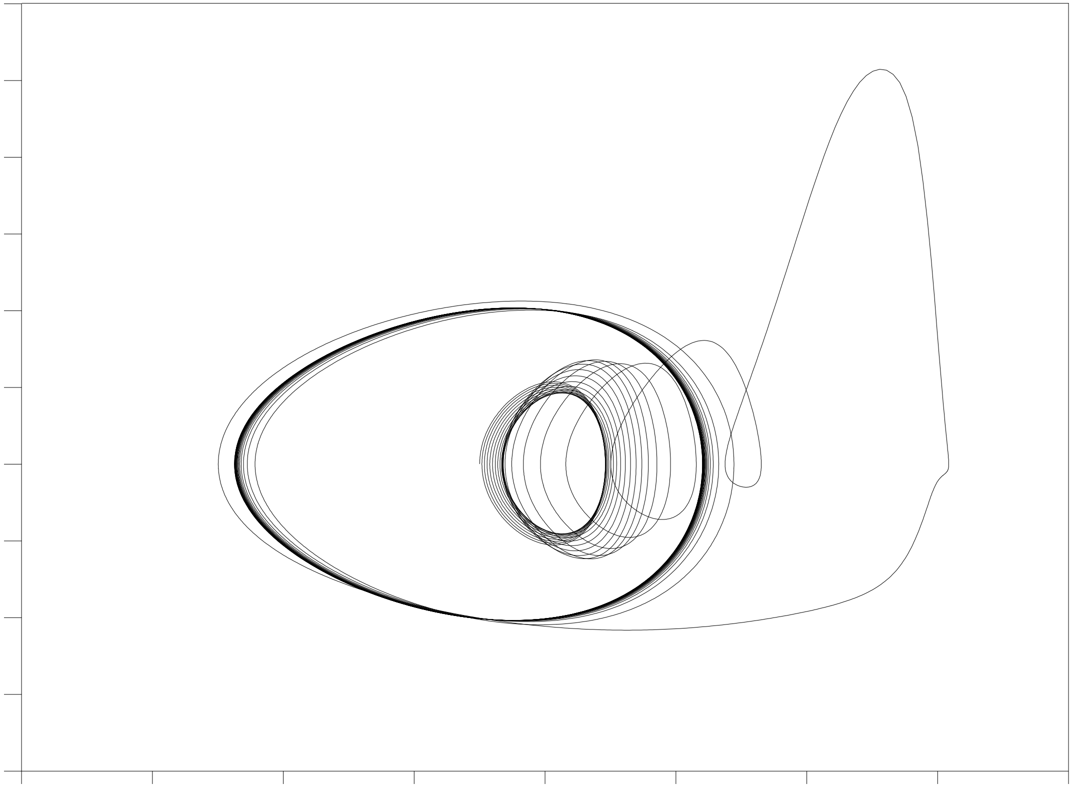
The importance of intermediate hypersurface

1. Possible change of coordinates
2. Taking care of quantum jumps
3. Separating different channels
4. Use of approximate methods

Transition from one channel to another



Elastic motion



All hopes for speed - up are now in

$$G(P_* X) = \int DP\, DX\, exp\{-i/h \;\; P_* X_* + i/h\, S|_* + i/h\, Q_*(Y_0 - Y_*)\ \}$$

There are three approaches, that show this expression to be mathematically correct without

Feynman reasoning

What can we do with this?

To make canonical transformation
with Generator F

$$H(P,X) \to H\left(X, \frac{\partial F}{\partial X}\right) + \frac{\partial F}{\partial t}$$

Most effective way is to choose final H = 0

$$H(P,X) \longrightarrow H(Q,Y) = H\left(X, \frac{\partial F_1}{\partial t}\right) + \left.\frac{\partial F_1}{\partial t}\right|_{Q,Y}$$

$$S = -P_* X_* + \int dF_1 + \int Q\,dY$$

As a result, we have functional delta function

$$G(P_*X) = exp\{- i/h \ \ P_*X + i/h \, F_1|_* + i/h \, Q_*(Y_0 - Y_*)\}$$

This is correct for real vector fields

For complex fields we have to find four generators

The final result is

$$A(P_i \to P_f) = \int dX_0 C\delta(X_0 P_0)\boldsymbol{exp}\{i/h\left(P_f X_f - P_i X_i\right) +$$

$$i/hF_1\Big|_* + i/hQ_i(Y_0 - Y_i) + i/hQ_f(Y_f - Y_0)\}$$

$$F_1: \quad H\left(X, \frac{\partial F_1}{\partial x}\right) = E$$

Look at this from the point of view of HPC

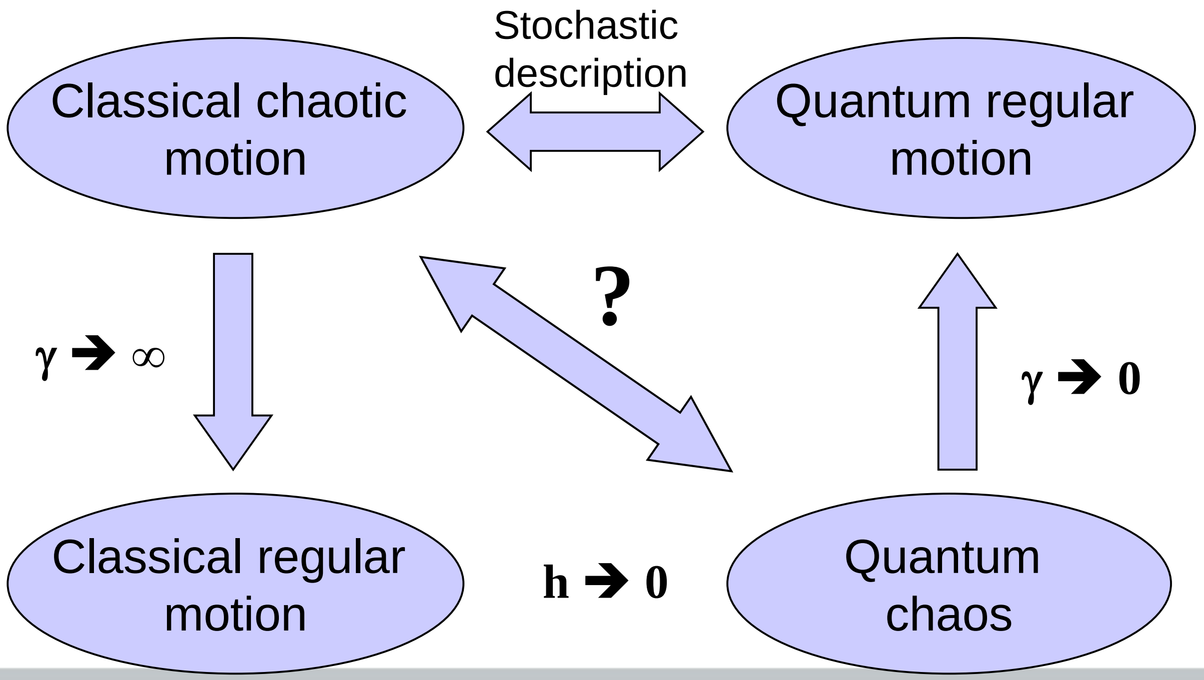
1. You have an integral with up to four PDE of the first order

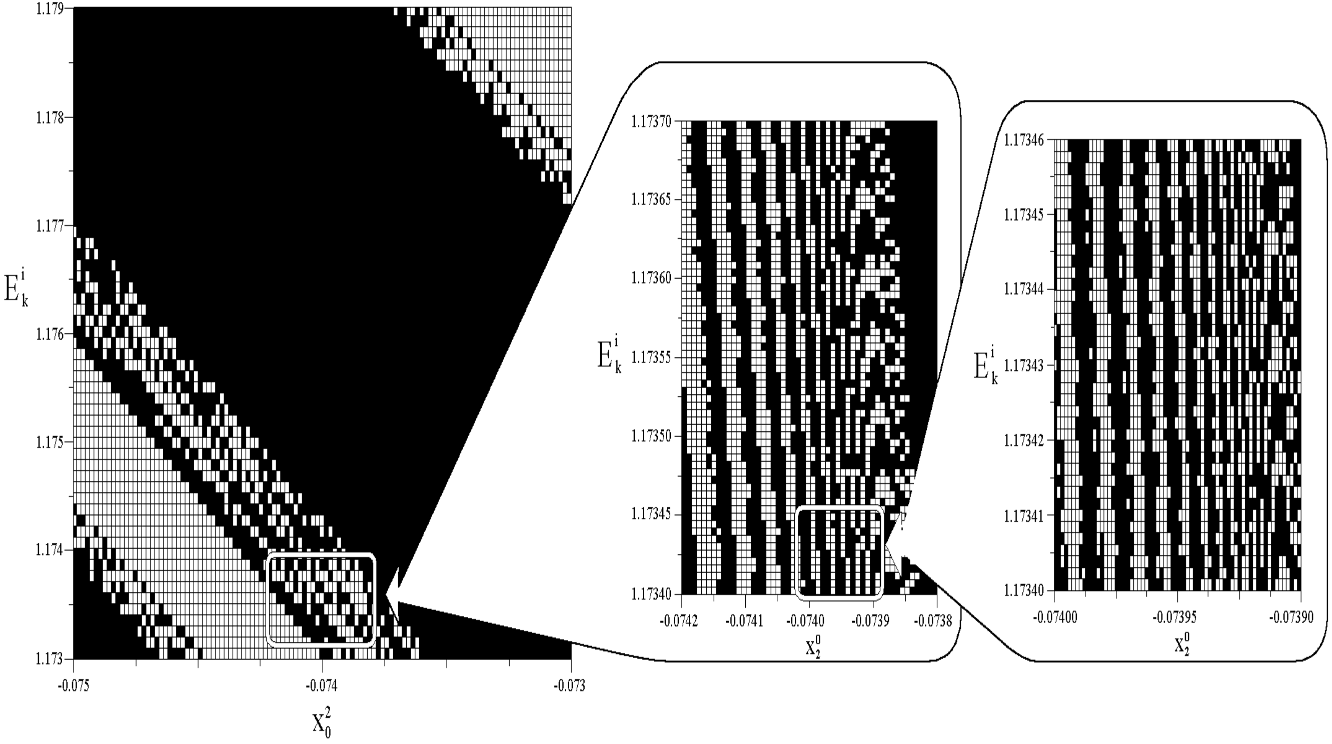
2. Nothing can be more parallel

3. PDE of the first order is equivalent to the system of the ODE

4. Algorithm is well suited for hybrid system

Problem of dynamic quantum chaos





1.179
1.178
1.177
1.176
1.175
1.174
1.173
E_k^i
-0.075
-0.074
-0.073
X_0^2
1.17370
1.17365
1.17360
1.17355
1.17350
1.17345
1.17340
E_k^i
-0.0742
-0.0741
-0.0740
-0.0739
-0.0738
x_2^0
1.17346
1.17345
1.17344
1.17343
1.17342
1.17341
1.17340
E_k^i
-0.07400
-0.07395
-0.07390
x_2^0

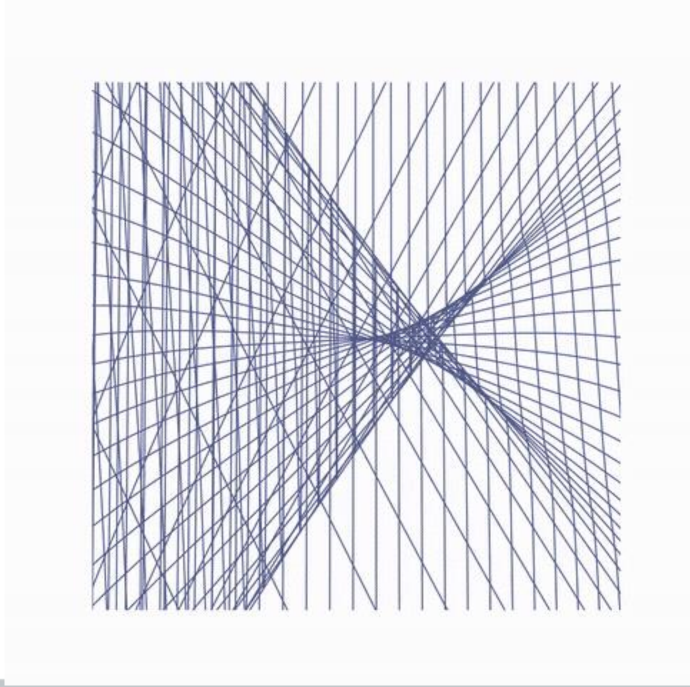
Before computations to make preliminary analysis

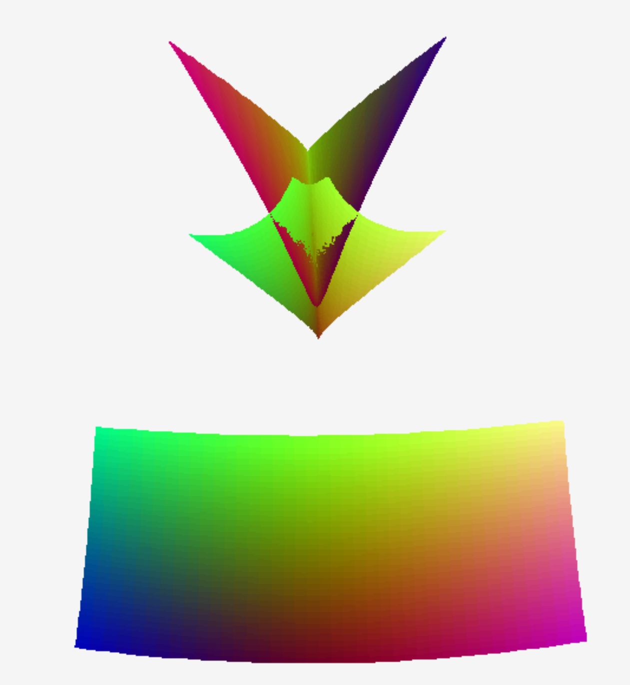
1. To use catastrophe theory

2. To choose one of the Toma elementary catastrophe

3. To make representation of the integral via one of functions, connected to elementary catastrophes

See couple of examples





Does it like an qualitative theory of PDE

If it is not, I will be surprised

To move forward, we have

1. To build functional representation for othe PDE.

2. To find proper procedures for reduction

Thank you for attention!

1. It was my personal opinion
2. I can very well agree to other opinions
3. Only discussion will generate ideal approach