Development of finite element method schemes for the study of collective models of atomic nuclei

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  - Eigenvalue problem
  - Metastable state problem
  - Multichannel Scattering Problem
- Test example
- Tasks

Applications

- Sub-barrier reactions of the fusion of heavy ions
- Study of geometric collective models of atomic nuclei

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The statement of the problem (BVP)

A self-adjoint elliptic PDE in the region $z = (z_1, ..., z_d) \in \Omega \subset \mathcal{R}^d$ (Ω is polyhedra)

$$\left(-\frac{1}{g_0(z)}\sum_{ij=1}^{d}\frac{\partial}{\partial z_i}g_{ij}(z)\frac{\partial}{\partial z_j}+V(z)-E\right)\Phi(z)=0, \quad g_0(z)>0, \quad g_{ji}(z)=g_{ij}(z).$$

Boundary conditions

$$\text{(Dirichlet)}: \qquad \Phi(z)|_S = 0,$$

$$\text{(Neumann)}: \qquad \left.\frac{\partial\Phi(z)}{\partial n_D}\right|_S = 0, \quad \frac{\partial\Phi(z)}{\partial n_D} = \sum_{ij=1}^{d}(\hat{n},\hat{e}_i)g_{ij}(z)\frac{\partial\Phi(z)}{\partial z_j},$$

$$\text{(Robin)}: \qquad \left.\frac{\partial\Phi(z)}{\partial n_D}\right|_S + \sigma(s)\Phi(z)\Big|_S = 0,$$

$\dfrac{\partial\Phi_m(z)}{\partial n_D}$ is the derivative along the conormal direction
$\hat{n}$ is the outer normal to the boundary of the domain $\partial\Omega$.

Ladyzhenskaya, O. A., The Boundary Value Problems of Mathematical Physics, Applied Mathematical Sciences, 49, (Berlin, Springer, 1985).
Shaidurov, V.V. Multigrid Methods for Finite Elements (Springer, 1995).

The statement of the problem

Conditions of normalization and orthogonality (for discrete spectrum problem)

$$\langle \Phi_m(z)|\Phi_{m'}(z)\rangle = \int\limits_{\Omega} dz g_0(z)\Phi_m(z)\Phi_{m'}(z) = \delta_{mm'}, \quad dz = dz_1 ... dz_d.$$

The FEM solution of the BVP is reduced to the determination of stationary points of the variational functional

$$\Xi(\Phi_m, E_m, z) \equiv \int\limits_{\Omega} dz g_0(z)\Phi_m(z)\,(D - E_m)\,\Phi(z) = \Pi(\Phi_m, E_m, z) - \oint_S \Phi_m(z)\frac{\partial \Phi_m(z)}{\partial n_D},$$

$$\Pi(\Phi_m, E_m, z) = \int\limits_{\Omega} dz \left[\sum_{ij=1}^{d} g_{ij}(z)\frac{\partial \Phi_m(z)}{\partial z_i}\frac{\partial \Phi_m(z)}{\partial z_j} + g_0(z)\Phi_m(z)(V(z) - E_m)\Phi_m(z)\right].$$

Strang, G., Fix, G.J.: An Analysis of the Finite Element Method, Prentice-Hall, Englewood Cliffs, New York (1973)

The expansion of the solution in the basis of piecewise polynomial functions $N_l^{p'}$

$$\Phi_m^h(z) = \sum_{l=1}^{L} N_l^{p'}(z)\Phi_{lm}^h,$$

Algebraic (eigenvalue) problem

$$(\mathbf{A} - \mathbf{B}E_m^h)\boldsymbol{\Phi}_m^h = 0, \tag{1}$$

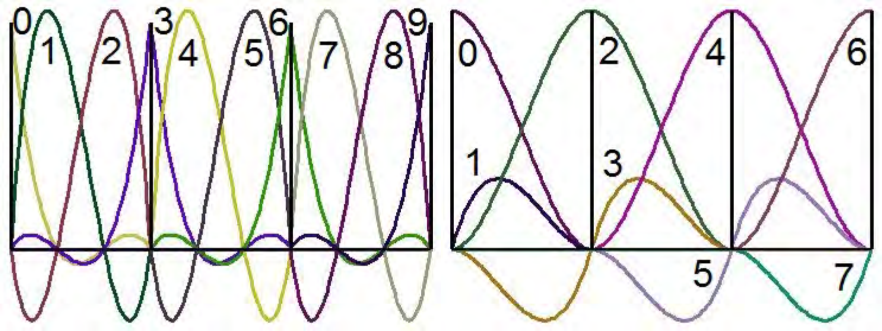
$$A_{ll'}^{p'} = \sum_{i,j=1}^{d} \int_\Omega \frac{\partial N_l^{p'}(z)}{\partial z_i} \frac{\partial N_{l'}^{p'}(z)}{\partial z_j} g_{ij}(z)dz - \oint_S N_l^{p'}(z)\frac{\partial N_{l'}^{p'}(z)}{\partial n_D} ds$$

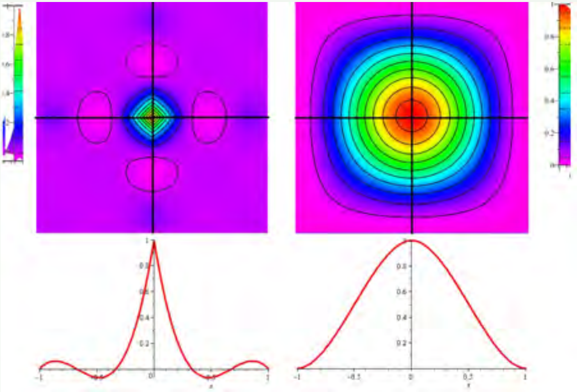
$$+ \int_\Omega N_l^{p'}(z)N_{l'}^{p'}(z)U(z)\, g_0(z)dz,$$

$$B_{ll'}^{p'} = \int_\Omega N_l^{p'}(z)N_{l'}^{p'}(z)g_0(z)dz. \tag{2}$$

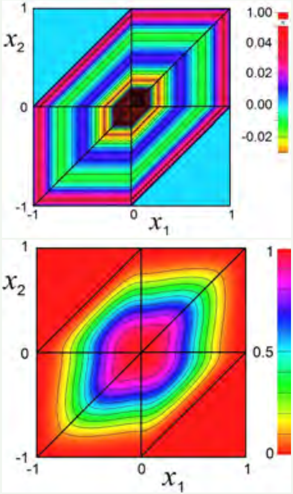
How piecewise polynomial functions $N_l^{p'}$ are obtained in FEM

- The polyhedral domain $\bar{\Omega} \subset \mathcal{R}^d$ is decomposed $\bar{\Omega} = \bar{\Omega}_h(z) = \bigcup_{q=1}^{Q} \Delta_q$ in finite elements in the form of d dimensional simplexes or hypercubes.
- On each finite element HIPs or LIPs $\varphi_{rq}^{\kappa p'}(z)$, $z \in \mathcal{R}^d$ are constructed.
- The piecewise polynomial functions $N_l^{p'}(z) \in C^{\kappa^c}$ are constructed by matching of the polynomials $\varphi_{rq}^{\kappa p'}(z)$





The piecewise 1D and 2D polynomials on domains $[-1, 1]$ and $[-1, 1] \times [-1, 1]$ equals one in origin obtained by matching of HIP(1,0) on $[-1, 0]$ with HIP(0,0) on $[0, 1]$ and by matching of LIP(3,0) on $[-1, 0]$ with LIP(0,0) on $[0, 1]$.



The piecewise 2D pols. obtained by matching of triangular LIPs and HIPs.

The basis functions constructed by matching d-dimensional HIPs has continuous partial first derivatives in boundaries of elements of a finite element grid.

Finite Element Method

Stages:

- BVP $\rightarrow$ minimization of quadratic functional problem
- Finite Element Mesh
- Construction of shape functions
  - Interpolation Polynomials
    - Lagrange Interpolation Polynomials
    - Hermite Interpolation Polynomials
  - ...
- Construction of piecewise polynomial functions by joining the shape functions
- Calculations of the integrals
  - Gaussian quadratures
  - ...
- Solving of Algebraic (Eigenvalue) Problem
  - Continuous Analog of Newton Method
  - ...

Problem statement

Self-adjoint system of N second-order ODEs for unknowns $\mathbf{\Phi}(z) \equiv \{\mathbf{\Phi}^{(i)}(z)\}_{i=1}^{N_o}$, $\mathbf{\Phi}^{(i)}(z) = (\Phi_1^{(i)}(z), \ldots, \Phi_N^{(i)}(z))^T$ by z in the region $z \in \Omega_z = (z^{\min}, z^{\max})$

$$\left(-\frac{1}{f_B(z)}\mathbf{I}\frac{d}{dz}f_A(z)\frac{d}{dz} + \mathbf{V}(z) + \frac{f_A(z)}{f_B(z)}\mathbf{Q}(z)\frac{d}{dz} + \frac{1}{f_B(z)}\frac{d\, f_A(z)\mathbf{Q}(z)}{dz} - E\,\mathbf{I}\right)\mathbf{\Phi}(z) = 0.$$

$f_B(z) > 0$ $f_A(z) > 0$, $\mathbf{I}$ is unit matrix; $\mathbf{V}(z)$ and $\mathbf{Q}(z)$ are a symmetric and an antisymmetric $N \times N$ matrices, with real or complex-valued coefficients from the Sobolev space $\mathcal{H}_2^{s\geq 1}(\Omega)$.

All coefficients are continuous (or piecewise continuous) functions that have derivatives up to the order of $\kappa^{\max} - 1 \geq 1$ in the domain $z \in \bar{\Omega}_z$.

The boundary conditions:

$$(\mathrm{I}): \quad \mathbf{\Phi}(z^t) = 0, \quad t = \min \text{ and/or} \max,$$

$$(\mathrm{II}): \quad \lim_{z \to z^t} f_A(z)\left(\mathbf{I}\frac{d}{dz} - \mathbf{Q}(z)\right)\mathbf{\Phi}(z) = 0, \quad t = \min \text{ and/or} \max,$$

$$(\mathrm{III}): \quad \lim_{z \to z^t} \left(\mathbf{I}\frac{d}{dz} - \mathbf{Q}(z)\right)\mathbf{\Phi}(z) = \mathbf{G}(z^t)\mathbf{\Phi}(z^t), \quad t = \min \text{ and/or} \max.$$

Problem 1. For bound or metastable states

Case of the real potentials and real eigenvalues E: $E_1 \leq E_2 \leq \ldots \leq E_{N_o}$

$$\langle \mathbf{\Phi}_m | \mathbf{\Phi}_{m'} \rangle = \int_{z^{\min}}^{z^{\max}} f_B(z) (\mathbf{\Phi}^{(m)}(z))^\dagger \mathbf{\Phi}^{(m')}(z) dz = \delta_{mm'}.$$

Case of the complex potentials and complex eigenvalues $E = \Re E + \imath \Im E$: $\Re E_1 \leq \Re E_2 \leq \ldots \leq \Re E_{N_o}$,

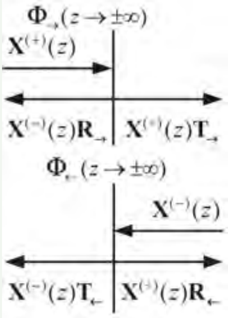
The eigenfunctions $\mathbf{\Phi}_m(z)$ obey the normalization and orthogonality conditions

$$(\mathbf{\Phi}_m | \mathbf{\Phi}_{m'}) = \int_{z^{\min}}^{z^{\max}} f_B(z) (\mathbf{\Phi}^{(m)}(z))^T \mathbf{\Phi}^{(m')}(z) dz = \delta_{mm'}.$$

J.G. Muga, J.P. Palao, B. Navarro, I.L. Egusquiza Complex absorbing potentials Physics Reports 395 (2004) 357–426
A.A. Gusev et al,Symbolic-numeric solution of boundary-value problems for the Schrodinger equation using the finite element method: scattering problem and resonance states, Lecture Notes in Computer Science 9301 (2015) 182–197.

Problem 2. The scattering problem

“incident wave + outgoing waves” asymptotic form



$$\mathbf{\Phi}_{\rightarrow}(z \rightarrow \pm\infty) = \begin{cases} \mathbf{X}^{(\rightarrow)}_{\min}(z) + \mathbf{X}^{(\leftarrow)}_{\min}(z)\mathbf{R}_{\rightarrow} + \mathbf{X}^{(c)}_{\min}(z)\mathbf{R}^{c}_{\rightarrow}, & z \rightarrow -\infty \\ \mathbf{X}^{(\rightarrow)}_{\max}(z)\mathbf{T}_{\rightarrow} + \mathbf{X}^{(c)}_{\max}(z)\mathbf{T}^{c}_{\rightarrow}, & z \rightarrow +\infty \end{cases}$$

$$\mathbf{\Phi}_{\leftarrow}(z \rightarrow \pm\infty) = \begin{cases} \mathbf{X}^{(\leftarrow)}_{\min}(z)\mathbf{T}_{\leftarrow} + \mathbf{X}^{(c)}_{\min}(z)\mathbf{T}^{c}_{\leftarrow}, & z \rightarrow -\infty \\ \mathbf{X}^{(\leftarrow)}_{\max}(z) + \mathbf{X}^{(\rightarrow)}_{\max}(z)\mathbf{R}_{\leftarrow} + \mathbf{X}^{(c)}_{\max}(z)\mathbf{R}^{c}_{\leftarrow}, & z \rightarrow +\infty \end{cases}$$

$\mathbf{\Phi}_{\rightarrow}(z)$, $\mathbf{\Phi}_{\leftarrow}(z)$ are the matrix solutions by dimension $N \times N^{L}_{o}$, $N \times N^{R}_{o}$

N^{L}_{o}, N^{R}_{o} are the numbers of open channels,

$\mathbf{X}^{(\rightarrow)}_{\min}(z)$, $\mathbf{X}^{(\leftarrow)}_{\min}(z)$ are open channel asymptotic solutions at $z \rightarrow -\infty$, dim. $N \times N^{L}_{o}$,

$\mathbf{X}^{(\rightarrow)}_{\max}(z)$, $\mathbf{X}^{(\leftarrow)}_{\max}(z)$ are open channel asymptotic solutions at $z \rightarrow +\infty$, dim. $N \times N^{R}_{o}$,

$\mathbf{X}^{(c)}_{\min}(z)$, $\mathbf{X}^{(c)}_{\max}(z)$ are closed channel solutions, dim. $N \times (N - N^{L}_{o})$, $N \times (N - N^{R}_{o})$,

$\mathbf{R}_{\rightarrow}$, $\mathbf{R}_{\leftarrow}$ are the reflection amplitude square matrices of dimension $N^{L}_{o} \times N^{L}_{o}$, $N^{R}_{o} \times N^{R}_{o}$,

$\mathbf{T}_{\rightarrow}$, $\mathbf{T}_{\leftarrow}$ are the transmission amplitude rectangular mat. of dim. $N^{R}_{o} \times N^{L}_{o}$, $N^{L}_{o} \times N^{R}_{o}$,

$\mathbf{R}^{c}_{\rightarrow}$, $\mathbf{T}^{c}_{\rightarrow}$, $\mathbf{T}^{c}_{\leftarrow}$, $\mathbf{R}^{c}_{\leftarrow}$ are auxiliary matrices.

Problem 2. The scattering problem

Wronskian conditions

$$\mathbf{Wr}(\mathbf{Q}(z);\mathbf{X}^{(\mp)}(z),\mathbf{X}^{(\pm)}(z)) = \pm 2\imath \mathbf{I}_{oo},\ \ \mathbf{Wr}(\mathbf{Q}(z);\mathbf{X}^{(\pm)}(z),\mathbf{X}^{(\pm)}(z)) = \mathbf{0}$$

$$\mathbf{Wr}(\mathbf{Q}(z);\mathbf{a}(z),\mathbf{b}(z)) = \mathbf{a}^T(z)\left(\frac{d\mathbf{b}(z)}{dz} - \mathbf{Q}(z)\mathbf{b}(z)\right) - \left(\frac{d\mathbf{a}(z)}{dz} - \mathbf{Q}(z)\mathbf{a}(z)\right)^T \mathbf{b}(z).$$

For real-valued potentials

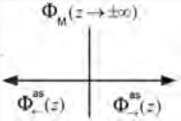
$$\mathbf{T}_{\rightarrow}^{\dagger}\mathbf{T}_{\rightarrow} + \mathbf{R}_{\rightarrow}^{\dagger}\mathbf{R}_{\rightarrow} = \mathbf{I}_{oo},\quad \mathbf{T}_{\leftarrow}^{\dagger}\mathbf{T}_{\leftarrow} + \mathbf{R}_{\leftarrow}^{\dagger}\mathbf{R}_{\leftarrow} = \mathbf{I}_{oo},$$
$$\mathbf{T}_{\rightarrow}^{\dagger}\mathbf{R}_{\leftarrow} + \mathbf{R}_{\rightarrow}^{\dagger}\mathbf{T}_{\leftarrow} = \mathbf{0},\quad \mathbf{R}_{\leftarrow}^{\dagger}\mathbf{T}_{\rightarrow} + \mathbf{T}_{\leftarrow}^{\dagger}\mathbf{R}_{\rightarrow} = \mathbf{0},$$
$$\mathbf{T}_{\rightarrow}^{T} = \mathbf{T}_{\leftarrow},\quad \mathbf{R}_{\rightarrow}^{T} = \mathbf{R}_{\rightarrow},\quad \mathbf{R}_{\leftarrow}^{T} = \mathbf{R}_{\leftarrow}.$$

For real-valued potentials the scattering matrix is symmetric and unitary, for complex potentials it is only symmetric

$$\mathbf{S} = \begin{pmatrix} \mathbf{R}_{\rightarrow} & \mathbf{T}_{\leftarrow} \\ \mathbf{T}_{\rightarrow} & \mathbf{R}_{\leftarrow} \end{pmatrix},\qquad \mathbf{S}^{\dagger}\mathbf{S} = \mathbf{S}\mathbf{S}^{\dagger} = 1.$$

Problem 3. The metastable state pr. with complex e.v. $E = \Re E + \imath \Im E$:

Asymptotic form



$$\mathbf{\Phi}_{\rightarrow}(z\to\pm\infty) = \begin{cases} \mathbf{X}^{(\leftarrow)}_{\min}(z)\mathbf{O}_{\leftarrow} + \mathbf{X}^{(c)}_{\min}(z)\mathbf{O}^{c}_{\leftarrow}, & z\to-\infty \\ \mathbf{X}^{(\rightarrow)}_{\max}(z)\mathbf{O}_{\rightarrow} + \mathbf{X}^{(c)}_{\max}(z)\mathbf{O}^{c}_{\rightarrow}, & z\to+\infty \end{cases}$$

Robin (Siegert) BC

(III) :

$$\lim_{z\to z^t}\left(\mathbf{I}\frac{d}{dz} - \mathbf{Q}(z)\right)\mathbf{\Phi}(z) = \mathbf{G}(z^t)\mathbf{\Phi}(z^t), \quad t = \min \text{ and/or } \max$$

$$\mathbf{G}(z^t) = \left(\lim_{z\to z^t}\left(\mathbf{I}\frac{d}{dz} - \mathbf{Q}(z)\right)\left(\mathbf{X}^{(\leftrightarrows)}_t(z), \mathbf{X}^{(c)}_t(z)\right)\right)\left(\mathbf{X}^{(\leftrightarrows)}_t(z), \mathbf{X}^{(c)}_t(z)\right)^{-1}$$

Orthonormalization conditions

$$(\mathbf{\Phi}_m|\mathbf{\Phi}_{m'}) = \int f_B(z)(\mathbf{\Phi}^{(m)}(z))^T\mathbf{\Phi}^{(m')}(z)dz = \delta_{mm'}.$$

J.G. Muga, J.P. Palao, B. Navarro, I.L. Egusquiza Complex absorbing potentials Physics Reports 395 (2004) 357–426

Test example (ODE System with Piecewise Constant Potentials)

$$\left(-\mathbf{I}\frac{d^2}{dz^2}+\mathbf{V}(z)-E\,\mathbf{I}\right)\boldsymbol{\Phi}(z)=0,\quad \mathbf{V}(z)=\{\mathbf{V}_1, z\le z_1, ..., \mathbf{V}_{k-1}, z\le z_{k-1}, \mathbf{V}_k, z>z_{k-1}\},$$

Matching the Fundamental Solutions

$$\left(-\mathbf{I}\frac{d^2}{dz^2}+\mathbf{V}_m-E\,\mathbf{I}\right)\boldsymbol{\Phi}_m(z)=0,\quad z\in(z_{m-1},z_m],\quad m=1,...,k,$$

$$\Rightarrow\quad \boldsymbol{\Phi}_m(z)=\sum_{i=1}^{N}\left(A_i^{(m)}\exp(-\sqrt{\lambda_i^{(m)}-E}z)\boldsymbol{\Psi}_i^{(m)}+B_i^{(m)}\exp(\sqrt{\lambda_i^{(m)}-E}z)\boldsymbol{\Psi}_i^{(m)}\right),$$

Here $\lambda_i^{(m)}$ and $\boldsymbol{\Psi}_i^{(m)}$ are the solutions of the algebraic eigenvalue problems

$$\mathbf{V}^{L,R}\boldsymbol{\Psi}_i^{(m)}=\lambda_i^{(m)}\boldsymbol{\Psi}_i^{(m)},\quad (\boldsymbol{\Psi}_i^{(m)})^T\boldsymbol{\Psi}_j^{(m)}=\delta_{ij}.$$

$$\lim_{z\to z_{m-1}}\boldsymbol{\Phi}_{m-1}(z)-\boldsymbol{\Phi}_m(z)=0,\quad \lim_{z\to z_{m-1}}\frac{\boldsymbol{\Phi}_{m-1}(z)}{dz}-\frac{\boldsymbol{\Phi}_m(z)}{dz}=0,\quad m=2,...,k$$

$\Rightarrow 2N(k-1)$ linear eqs. with $2N(k-1)$ unknowns.

Problem 2. The scattering problem. Example of asymptotic solutions

ODE in asymptotic regions $z \to \pm\infty$

$$\left(-\mathbf{I}\frac{d^2}{dz^2} + \mathbf{V}^{L,R} - E\,\mathbf{I}\right)\boldsymbol{\Phi}(z) = 0, \quad \text{where } \mathbf{V}^{L,R} \text{ are constant matrices.}$$

Asymptotic solutions

The open channel asymptotic solutions: $i_o = 1, ..., N_o^{L,R}$:

$$\mathbf{X}_{i_o}^{(\rightleftarrows)}(z \to \pm\infty) \to \frac{\exp\left(\pm\imath\sqrt{E - \lambda_{i_o}^{L,R}}z\right)}{\sqrt[4]{E - \lambda_{i_o}^{L,R}}}\boldsymbol{\Psi}_{i_o}^{L,R}, \quad \lambda_{i_o}^{L,R} < E.$$

The closed channels asymptotic solutions $i_c = N_o^{L,R} + 1, \dots, N$:

$$\mathbf{X}_{i_o}^{(c)}(z \to \pm\infty) \to \exp\left(-\sqrt{\lambda_{i_c}^{L,R} - E}|z|\right)\boldsymbol{\Psi}_{i_c}^{L,R}, \quad \lambda_{i_c}^{L,R} \geq E.$$

Here $\lambda_i^{L,R}$ and $\boldsymbol{\Psi}_{i_c}^{L,R}$ are the solutions of the algebraic eigenvalue problems

$$\mathbf{V}^{L,R}\boldsymbol{\Psi}_i^{L,R} = \lambda_i^{L,R}\boldsymbol{\Psi}_i^{L,R}, \quad (\boldsymbol{\Psi}_i^{L,R})^T\boldsymbol{\Psi}_j^{L,R} = \delta_{ij}.$$

Problem 3. The metastable state pr. with complex e.v. $E = \Re E + \imath \Im E$:

Example of asymptotic solutions

The open channel asymptotic solutions: $i_o = 1, ..., N_o^{L,R}$:

$$\mathbf{X}_{i_o}^{(\rightleftarrows)}(z \to \infty) \to \exp\left(+\imath\sqrt{E - \lambda_{i_o}^{L,R}}|z|\right)\mathbf{\Psi}_{i_o}^{L,R}, \quad \lambda_{i_o}^{L,R} < \Re E, \quad i_o = 1, ..., N_o^{L,R},$$

The closed channels asymptotic solutions $i_c = N_o^{L,R} + 1, \ldots, N$:

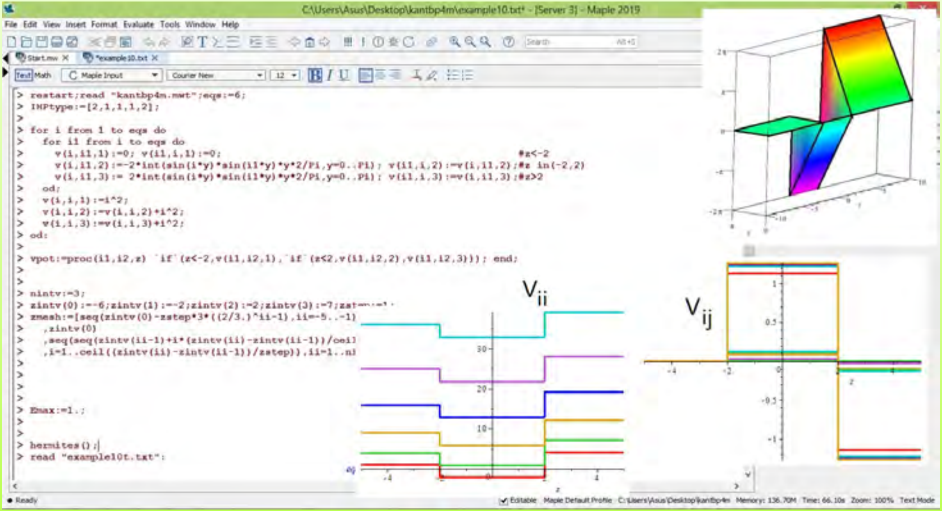
$$\mathbf{X}_{i_c}^{(c)}(z \to \infty) \to \exp\left(-\sqrt{\lambda_{i_c}^{L,R} - E}|z|\right)\mathbf{\Psi}_{i_c}^{L,R}, \quad \lambda_{i_c}^{L,R} \geq \Re E, \quad i_c = N_o^{L,R} + 1, \ldots, N.$$

Robin BC

$$\mathcal{R}(z^t) = \mathbf{\Psi}^{L,R}\mathbf{F}^{L,R}\left(\mathbf{\Psi}^{L,R}\right)^{-1},$$

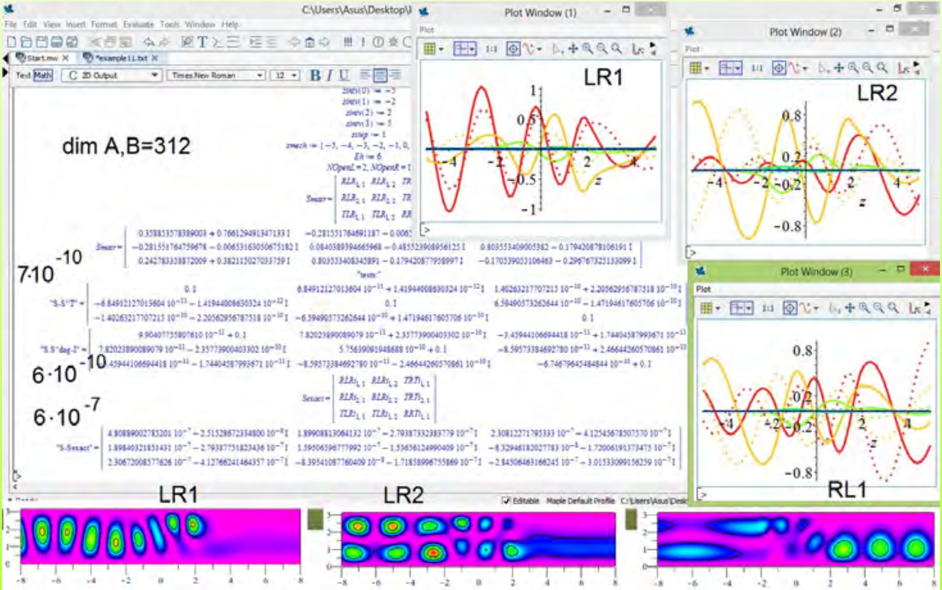
$$\mathbf{F}^{L,R} = \mathrm{diag}(..., \pm\sqrt{\lambda_{i_c}^{L,R} - E}, ..., \mp\imath\sqrt{E - \lambda_{i_o}^{L,R}}, ...)$$

The piecewise constant potentials

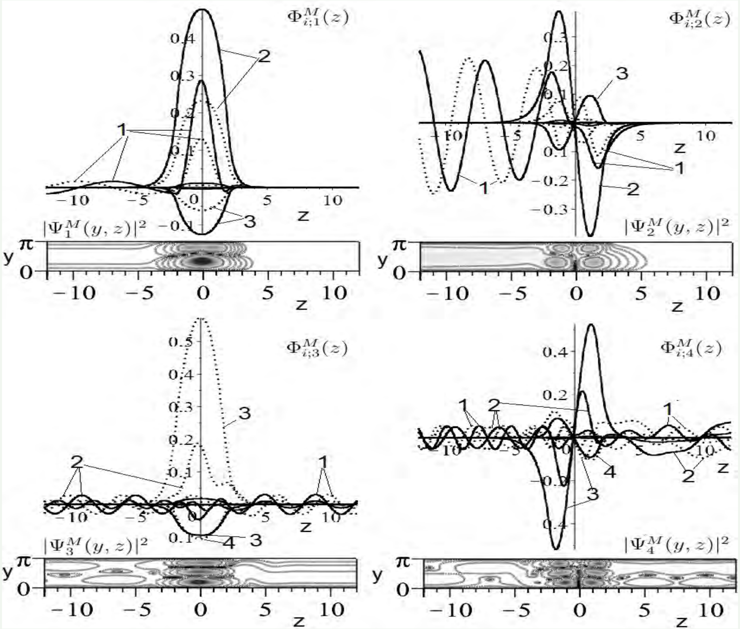


A. Gusev, S. Vinitsky, V. Gerdt, O. Chuluunbaatar, G. Chuluunbaatar, L. Le Hai, E. Zima, A Maple implementation of the finite element method for solving boundary problems of the systems of ordinary second order differential equations. Maple Conference, Waterloo Maple Inc., Canada 2020

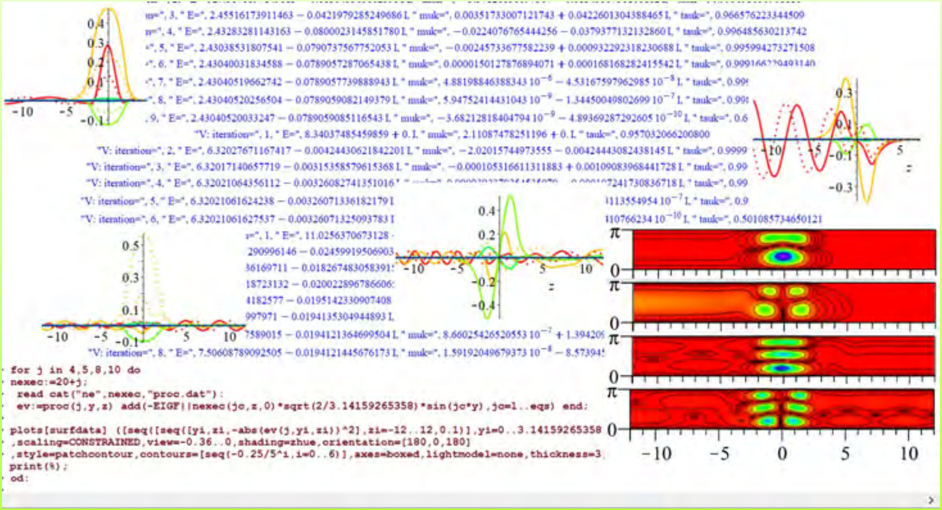
The piecewise constant potentials (multichannel scattering problem)



The piecewise constant potentials (resonance scattering states)

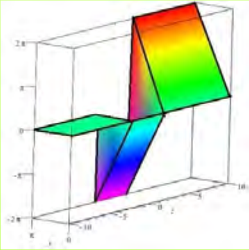


The piecewise constant potentials (metastable state problem)



Задание на бакалаврскую или магистерскую работу

- Решить
  - многоканальную задачу рассеяния
  - задачу на метастабильные состояния
- для
  - тестового примера (а)
  - задачи прохождения двух одномерных частиц с осцилляторным взаимодействием через барьер (б)
  - задачи рассеяния трёх одномерных частиц с потенциалом взаимодействия Морзе (в)
- с помощью МКЭ
  - с ИПЛ (или ИПЭ) на прямоугольной сетке (а,б)
  - с одномерными ИПЛ (или ИПЭ) и разложения по базисным функциям (в)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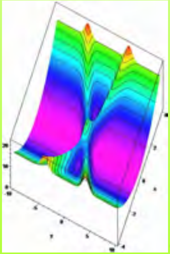
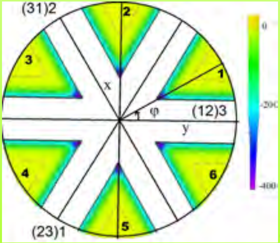

(б) или



(в)