Construction and application of fully symmetric quadrature rules on the simplexes

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OUTLINE

- Motivation and the statement of the problem
- Construction of fully symmetric Gaussian quadratures on simplexes:
  - No points outside the simplex
  - Positive weights
- Resume

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A detailed description in:
G. Chuluunbaatar, O. Chuluunbaatar, A.A. Gusev, S.I. Vinitsky,
PI-type fully symmetric quadrature rules on the 3-,..., 6-simplexes,
Computers & Mathematics with Applications 124, pp. 89–97 (2022).

Motivation

A realistic and quantized quadrupole-octupole-vibrational collective Hamiltonian

$$H_{\rm coll} = -\frac{\hbar^2}{2}\left\{\frac{1}{\det B_2}\sum_{\nu,\nu'=0,2}\frac{\partial}{\partial\alpha_{2\nu}}\sqrt{\det B_2}[B_2^{-1}]^{\nu\nu'}\frac{\partial}{\partial\alpha_{2\nu'}} + \frac{1}{\det B_3}\sum_{\nu,\nu'=0}^{3}\frac{\partial}{\partial\alpha_{3\nu}}\sqrt{\det B_3}[B_3^{-1}]^{\nu\nu'}\frac{\partial}{\partial\alpha_{3\nu'}}\right\}$$
$$+V(\alpha_{20},\alpha_{22},\alpha_{30},\alpha_{31},\alpha_{32},\alpha_{33})$$

α_{20}, α_{22}, α_{30}, α_{31}, α_{32}, α_{33} quadrupole and octupole collective variables with metrics;
$B_2 \equiv B_2(\alpha_{20},\alpha_{22})$, $B_3 \equiv B_3(\alpha_{30},\alpha_{31},\alpha_{32},\alpha_{33})$ denote the quadrupole and octupole microscopic mass tensor

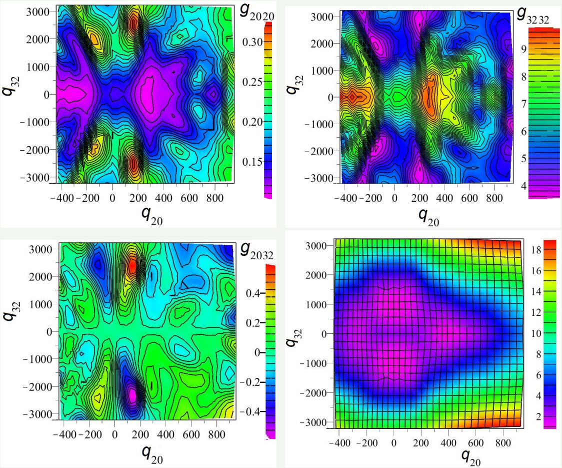
A. Dobrowolski, K. Mazurek, and A. Góźdź, Consistent quadrupole-octupole collective model. Phys. Rev. C 94, p. 054322 (2016)

A. Dobrowolski, K. Mazurek, and A. Góźdź, Rotational bands in the quadrupole-octupole collective model. Phys. Rev. C 97, p. 024321 (2018)

A.A. Gusev et al, Finite Element Method for Solving the Collective Nuclear Model with Tetrahedral Symmetry. Acta Physica Polonica B Proceedings Supplement 12, p. 589–594 (2019).

Motivation

Example: reduced 2D model ^{156}Dy nucleus



The coefficients $g_{ij}(x)$ and the potential energy $V(x_1, x_2)$ of ^{156}Dy nucleus given in variables (q_{20}, q_{32}) in units $10^{-5}\hbar^2/(\text{MeV fm}^5)$.

Motivation

Finite Element Method

- BVP $\rightarrow$ minimization of quadratic functional
- Finite Element Mesh (Simplex Mesh, Parallelepiped Mesh, ...)
- Construction of shape functions
  - Lagrange Interpolation Polynomials
  - Hermite Interpolation Polynomials
  - ...
- Construction of piecewise polynomials by joining the shape functions
- Calculations of the integrals
  (of the order $2p$ for FEM scheme of the order p).
  - Fully symmetric Gaussian quadratures
  - ...
- Solving of Algebraic Eigenvalue Problem

‘

Construction of the d-dimensional quadrature formulas

p-order QR for the master-element $\hat{x}_j = (\hat{x}_{j1}, \ldots, \hat{x}_{jd})$, $\hat{x}_{jk} = \delta_{jk}$, $j = 0, \ldots, d$

$$\int_{\Delta_d} V(x)dx = \frac{1}{d!} \sum_{j=1}^{N_{dp}} w_j V(x_{j1}, \ldots, x_{jd}), x = (x_1, \ldots, x_d), \quad dx = dx_1 \ldots dx_d,$$

N_{dp} is the number of nodes, w_j are the weights, and $(x_{j1}, \ldots, x_{jd})$ are the nodes.

$$\int_{\Delta_d} x_1^{k_1} \cdots x_{d+1}^{k_{d+1}} dx = \frac{\prod_{i=1}^{d+1} k_i!}{\left(d + \sum_{i=1}^{d+1} k_i\right)!}, \quad x_{d+1} = 1 - \sum_{i=1}^{d} x_i.$$

Barycentric coordinates (BC) $(y_1, \ldots, y_{d+1})$, $\sum_{k=1}^{d+1} y_k = 1$.

$$\int_{\Delta_d} V(x)dx = \frac{1}{d!} \sum_{j=1} w_j \sum_{k_1, \ldots, k_{d+1}} V(y_{jk_1}, \ldots, y_{jk_d} | y_{jk_{d+1}}),$$

where the internal summation over $k_1, \ldots, k_{d+1}$ is carried out over the different permutations of the BC $(y_{j1}, \ldots, y_{jd+1})$.

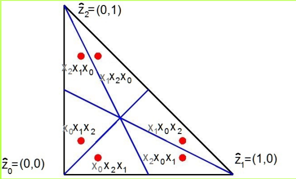
ORBITS

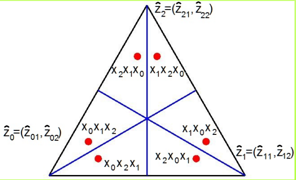
Orbit $S_{[i]} \equiv S_{m_1 \dots m_{r_{di}}}$

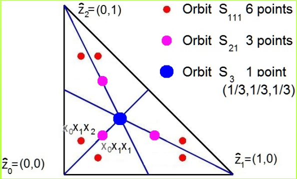
$$(y_1, \dots, y_{d+1}) = (\overbrace{\lambda_1, \dots, \lambda_1}^{m_1 \text{ times}}, \dots, \overbrace{\lambda_{m_{r_{di}}}, \dots, \lambda_{m_{r_{di}}}}^{m_{r_{di}} \text{ times}}),$$

$$\sum_{j=1}^{r_{di}} m_j = d+1, \quad \sum_{j=1}^{r_{di}} m_j \lambda_j = 1, \quad m_1 \geq \dots \geq m_{r_{di}}.$$

$$P_{di} = \frac{(d+1)!}{m_1! \dots m_{r_{di}}!} \quad \text{is the number of different permutations.}$$







System of nonlinear algebraic equations w.r.t unknowns $W_{i,j}$ and $\lambda_{i,jl}$

$$\int_{\Delta_d} s_2^{l_2} s_3^{l_3} \times \cdots \times s_{d+1}^{l_{d+1}} dx = \frac{1}{d!} \sum_{i=0}^{M_d} P_{di} \sum_{j=1}^{K_{di}} W_{i,j} s_{i,j2}^{l_2} s_{i,j3}^{l_3} \times \cdots \times s_{i,jd+1}^{l_{d+1}}, \quad (1)$$

$$s_k = \sum_{l=1}^{d+1} x_l^k, \quad s_{i,jk} = \sum_{l=1}^{r_{di}} m_l \lambda_{i,jl}^k \quad 2l_2 + 3l_3 + \cdots + (d+1)l_{d+1} \leq p,$$

where P_{di} is the number of different permutations of the BC corresponded to the orbit $S_{[i]}$.

The minimal numbers E_{dp} of independent equations for fully symmetric p-order quadrature rules.

$d \backslash p$	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
2	4	5	7	8	10	12	14	16	19	21	24	27	30	33	37	40	44
3	5	6	9	11	15	18	23	27	34	39	47	54	64	72	84	94	108
4	5	7	10	13	18	23	30	37	47	57	70	84	101	119	141	164	192
5	5	7	11	14	20	26	35	44	58	71	90	110	136	163	199	235	282
6	5	7	11	15	21	28	38	49	65	82	105	131	164	201	248	300	364

Modified Levenberg-Marquardt method

The problem of solving the system of nonlinear equations

$$f_i(\mathbf{x}) = 0, \quad i = 1, \dots, m, \quad \mathbf{x} = (x_1, \dots, x_n) \in \mathcal{X},$$

and the corresponding minimization problem

$$\min_{\mathbf{x}\in\mathcal{X}} \frac{1}{2}\|F(\mathbf{x})\|^2 \equiv \min_{\mathbf{x}\in\mathcal{X}} \frac{1}{2}\sum_{i=1}^{m} f_i^2(\mathbf{x}),$$

where $\mathcal{X} \subseteq R^n$ is a nonempty, closed and convex set. LM-type algorithm is an iterate method which solves at each iteration a linearization subproblem with the form

$$\min_{\mathbf{x}^k+\mathbf{d}\in\mathcal{X}} F_k(\mathbf{d}), \quad F_k(\mathbf{d}) = \frac{1}{2}\|F(\mathbf{x}^k) + J_k\mathbf{d}\|^2 + \frac{1}{2}\mu_k(\mathbf{d}, D_k\mathbf{d}),$$

where $\mathbf{x}^k$ is the current iterate, $J_k \in R^{m\times n}$ is a Jacobian of $F(\mathbf{x})$ at $\mathbf{x} = \mathbf{x}^k$, $D_k = \mathrm{diag}(J_k^T J_k) \in R^{n\times n}$ is a positive diagonal matrix and μ_k is a positive parameter. Hence the solution $F_k(\mathbf{d})$ of subproblem (2) always exists uniquely, in particular for unconstrained case

$$\mathbf{d}^k = -(J_k^T J_k + \mu_k D_k)^{-1} J_k^T F(\mathbf{x}^k).$$

Algorithm for calculations

1. Choose $\mathbf{x}^0 \in \mathcal{X}$ and $\mu > 0$, and set $k = 0$.
2. If $\|F(\mathbf{x}^k)\| = 0$, stop.
3. Calculate J_k and set $\mu_k = \mu\|F(\mathbf{x}^k)\|^2$, and compute $\mathbf{d}^k$.
4. $\mathbf{x}^{k+1} = \mathbf{x}^k + \mathbf{d}^k$, $k = k + 1$, and go to 2.

Results

Set of quadrature formulas on a 6-simplex

p	N_{dp}	S_7	S_{61}	S_{52}	S_{43}	S_{511}	S_{421}	S_{331}	S_{322}
4	43	1	1		1				
5	64	1	1	1	1				
6	175		2	1	1		1		
7	252		2	1	2	1	1		
8	448		3		2	1	3		
9	700		2	2	3	2	1	1	1
10	1078		2	3	2	3	3	2	1

Results

The minimal numbers N_{dp} of nodes for PI-type fully symmetric p-order quadrature rules and comparison with the known numbers N_{dp}.

p	$d=3$		$d=4$		$d=5$		$d=6$	
	cur.	JS	cur.	F	cur.	G	cur.	G
4	14	14	20	20	27	27	43	43
6	24	24	56	56	102	102	175	175
8	46	46	105	105	228	257	448	553
10	79	81	210	210	479		1078	
12	123	168	370	445				
14	175	204	601	725				
16	248	304	956	1055				
18	343	436						
20	441	552						

JS: J. Jaśkowiec, N. Sukumar, Int. J. Num. Methods Eng. 122 (2021) 148–171.
F: C.V. Frontin et al, App. Num. Math. 166 (2021) 92–113.
G: A.A. Gusev et al, Lecture Notes in Computer Science 11077 (2018) 197–213.

Estimates of the errors of the quadrature rules

Decomposition the integrand $V(x)$ into a Taylor series

$$V(x)=V^t(x)+O(x^{p+2}),\ \ V^t(x)=\sum_{i_1+\ldots+i_d\leq p+1} V^{(i_1,\ldots,i_d)}(x_t)\frac{(x_1-x_{1t})^{i_1}\times\ldots\times(x_d-x_{dt})^{i_d}}{i_1!\times\ldots\times i_d!},$$

where $V^{(i_1,\ldots,i_d)}(x_t)$ is a mixed derivative at $x=x_t$.

Taking into account that the quadrature is exact for polynomials of degree less than p, one has

$$\varepsilon(V^t(x))\equiv\left|\int_{\Delta_d} V^t(x)dx-\frac{1}{d!}\sum_{j=1}^{N_{dp}} w_j V^t(x_{j1},\ldots,x_{jd})\right|$$

$$\leq\sum_{i_1+\ldots+i_d=p+1}|V^{(i_1,\ldots,i_d)}|\,\varepsilon_{i_1,\ldots,i_d},\quad \varepsilon_{i_1,\ldots,i_d}\equiv\varepsilon\left(\frac{x_1^{i_1}\times\ldots\times x_d^{i_d}}{i_1!\times\ldots\times i_d!}\right),$$

The largest of the coefficients, $\max \varepsilon_{i_1,\ldots,i_d}$, their sum $\sum \varepsilon_{i_1,\ldots,i_d}$ and the root of the sum of their squares $\sqrt{\sum \varepsilon^2_{i_1,\ldots,i_d}}$ for a 6-simplex.

p	N_{dp}	$\max \varepsilon_{i_1,\ldots,i_6}$	$\sum \varepsilon_{i_1,\ldots,i_6}$	$\sqrt{\sum \varepsilon^2_{i_1,\ldots,i_6}}$
4	43	$2.23 \cdot 10^{-9}$	$4.88 \cdot 10^{-9}$	$2.54 \cdot 10^{-9}$
5	64	$2.45 \cdot 10^{-10}$	$5.89 \cdot 10^{-10}$	$2.89 \cdot 10^{-10}$
6	175	$2.41 \cdot 10^{-12}$	$1.43 \cdot 10^{-11}$	$4.45 \cdot 10^{-12}$
7	252	$3.01 \cdot 10^{-13}$	$8.26 \cdot 10^{-13}$	$3.38 \cdot 10^{-13}$
8	448	$7.08 \cdot 10^{-15}$	$3.30 \cdot 10^{-14}$	$1.04 \cdot 10^{-14}$
9	700	$6.48 \cdot 10^{-16}$	$2.05 \cdot 10^{-15}$	$7.34 \cdot 10^{-16}$
10	1078	$3.99 \cdot 10^{-18}$	$3.30 \cdot 10^{-17}$	$7.19 \cdot 10^{-18}$

Test example

6D integral

$$I_d = \int_{\Delta_d} (x_1 + \ldots + x_6) \exp(-x_1 - \ldots - x_6) dx_1 \ldots dx_6 = 6 - \frac{1957}{120\, e} \approx 0.000499448.$$

The differences ϵ^q_{test}, between the numerical and exact values, and the corresponding Runge coefficient $\beta = \log_2 \left| (\epsilon^q_{\text{test}} - \epsilon^{2q}_{\text{test}}) / (\epsilon^{2q}_{\text{test}} - \epsilon^{4q}_{\text{test}}) \right|$

p	ϵ^2_{test}	ϵ^4_{test}	ϵ^8_{test}	β
4	$+7.91 \cdot 10^{-12}$	$+1.73 \cdot 10^{-13}$	$+2.90 \cdot 10^{-15}$	5.50
5	$+1.06 \cdot 10^{-12}$	$+1.81 \cdot 10^{-14}$	$+2.90 \cdot 10^{-16}$	5.87
6	$-1.73 \cdot 10^{-14}$	$-7.35 \cdot 10^{-17}$	$-2.93 \cdot 10^{-19}$	7.88
7	$-1.81 \cdot 10^{-16}$	$-8.02 \cdot 10^{-19}$	$-3.22 \cdot 10^{-21}$	7.82
8	$+2.09 \cdot 10^{-18}$	$+2.34 \cdot 10^{-21}$	$+2.35 \cdot 10^{-24}$	9.80
9	$-3.86 \cdot 10^{-20}$	$-5.12 \cdot 10^{-23}$	$-5.34 \cdot 10^{-26}$	9.56
10	$-1.18 \cdot 10^{-22}$	$-3.63 \cdot 10^{-26}$	$-9.35 \cdot 10^{-30}$	11.66

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INQSIM - a program for converting PI-type fully symmetric quadrature rules on 2-,..., 6-simplexes from compact to expanded forms

Authors: G.Chuluunbaatar, O.Chuluunbaatar, A.A.Gusev, S.I.Vinitsky

Languages: Maple, Fortran

The program is designed to construct d-dimensional p-ordered quadrature rules in expanded form for integration over the d-dimensional standard unit simplex Δ_d with the vertices $\hat{x}_j = (\hat{x}_{j1},\ldots,\hat{x}_{jd})$, $\hat{x}_{jk} = \delta_{jk}$, $j=0,\ldots d$, $k=1,\ldots d$,

$$\int_{\Delta_d} V(x)dx = |\Delta_d| \sum_{j=1}^{N_{dp}} w_j V(x_{j1},\ldots,x_{jd}), \quad x=(x_1,\ldots,x_d), \quad dx = dx_1\ldots dx_d,$$

where $|\Delta_d| = 1/d!$ is the volume of the simplex. Here N_{dp} is the number of nodes, w_j are the weights, and $(x_{j1},\ldots,x_{jd})$ are the nodes.

- A method for constructing fully symmetric Gaussian quadrature rules with positive weights, and with nodes lying inside the simplex is discussed.
- The quadrature rules up to 20-th order on the tetrahedron, 16-th order on 4-simplex, 10-th order on 5- and 6-simplexes are obtained.
- For the convenience of their use, the INQSIM program was created and presented in the JINR program library (JINRLIB).
- The developed method is oriented on solving the 6D elliptic BVP by the FEM for describing the discrete spectrum of the collective model of the atomic nucleus.

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THANK YOU FOR YOUR ATTENTION