Hermitian Finite Elements for Hypercube

A.A. Gusev
(Joint Institute for Nuclear Research, Dubna, Russia)

G. Chuluunbaatar, V.P. Gerdt, S.I. Vinitsky
(JINR, Dubna)
L.L. Hai (Ho Chi Minh city University of Education, Ho Chi Minh city, Vietnam)

OUTLINE

- The statement of the problem
- Lagrange & Hermite Finite Elements
  - 1d
  - Simplex FE
  - Hypercubical FE
- Example
- Resume

October 13, 2020, St. Petersburg

Polynomial Computer Algebra '2020

The statement of the problem

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

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

$g_0(z) > 0$, $g_{ji}(z) = g_{ij}(z)$ and $V(z)$ are the real-valued functions, continuous together with their derivatives to a given order.
+ Boundary conditions
+ Conditions of normalization and orthogonality (for discrete spectrum problem)

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).

Finite Element Method

Stages:

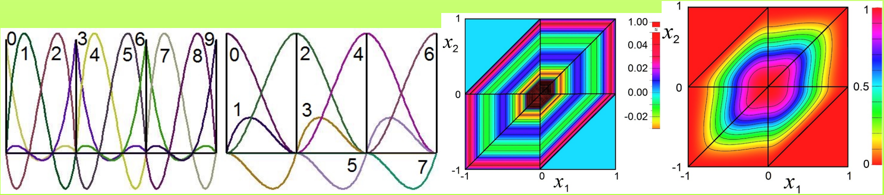
- Finite Element Mesh
  - Simplex Mesh
  - Parallelepiped Mesh
  - ...
- Construction of shape functions
  - Interpolation Polynomials
    - Lagrange Interpolation Polynomials
    - Hermite Interpolation Polynomials
  - ...
- Construction of piecewise polynomial functions by joining the shape functions
- Calculations of the integrals
  - Construction of fully symmetric Gaussian quadratures
    - No points outside the simplex
    - Positive weights
  - ...
- Solving of Algebraic Eigenvalue Problem

Lagrange Finite Elements

The polyhedron $\Omega = \bigcup_{q=1}^{Q} \Delta_q$ is covered with simplexes Δ_q with $d{+}1$ vertices:

$$\hat{z}_i = (\hat{z}_{i1}, \hat{z}_{i2}, ..., \hat{z}_{id}), \quad i = 0, ..., d.$$

On each simplex Δ_q we introduce the shape functions, for example IPL: $\varphi_r(\xi_{r'}) = \delta_{rr'}$.
The piecewise polynomial functions $N_l(z)$ are constructed by joining the shape functions $\varphi_l(z)$ in the simplex Δ_q: $N_l(z) = \left\{ \varphi_l(z), A_l \in \Delta_q; 0, A_l \notin \Delta_q \right\}$ and possess the following properties:
functions $N_l(z)$ are continuous in the domain Ω;
the functions $N_l(z)$ equal 1 in one of the points A_l and zero in the rest points.



Finite Element Method

Solutions $\hat{\Phi}(z)$ are sought in the form of a finite sum over the basis of local functions $N^g_\mu(z)$ in each nodal point $z = z_k$ of the grid $\Omega_h(z)$:

$$\hat{\Phi}(z) = \sum_{\mu=0}^{L-1} \Phi^h_\mu N^g_\mu(z),$$

where L is number of local functions, and Φ^h_μ are nodal values of function $\hat{\Phi}(z)$ at nodal points z_l.

After substituting the expansion into a variational functional and minimizing it, we obtain the generalized eigenvalue problem

$$\mathbf{A}^p \boldsymbol{\xi}^h = \varepsilon^h \mathbf{B}^p \boldsymbol{\xi}^h.$$

Here $\mathbf{A}^p$ is the stiffness matrix; $\mathbf{B}^p$ is the positive definite mass matrix; $\boldsymbol{\xi}^h$ is the vector approximating the solution on the finite-element grid; and ε^h is the corresponding eigenvalue.

1D Interpolation Hermite Polynomials

1D Interpolation Lagrange Polynomials

$$\varphi_r(z_{r'}) = \delta_{rr'}, \quad \varphi_r(z_{r'}) = \prod_{r'=0, r'\neq r}^{p} \left(\frac{z - z_{r'}}{z_r - z_{r'}} \right).$$

1D Interpolation Hermite Polynomials

$$\varphi_r^{\kappa}(z_{r'}) = \delta_{rr'}\delta_{\kappa 0}, \quad \left. \frac{d^{\kappa'}\varphi_r^{\kappa}(z)}{dz^{\kappa'}} \right|_{z=z_{r'}} = \delta_{rr'}\delta_{\kappa\kappa'}.$$

To calculate the IHPs we introduce the auxiliary weight function

$$w_r(z) = \prod_{r'=0, r'\neq r}^{p} \left(\frac{z - z_{r'}}{z_r - z_{r'}} \right)^{\kappa_{r'}^{\max}}, \qquad \frac{d^{\kappa} w_r(z)}{dz^{\kappa}} = w_r(z) g_r^{\kappa}(z), \qquad w_r(z_r) = 1,$$

$$g_r^{\kappa}(z) = \frac{d g_r^{\kappa-1}(z)}{dz} + g_r^1(z) g_r^{\kappa-1}(z), \quad g_r^0(z) = 1, \quad g_r^1(z) = \sum_{r'=0, r'\neq r}^{p} \frac{\kappa_{r'}^{\max}}{z - z_{r'}}.$$

Interpolation Hermite Polynomials

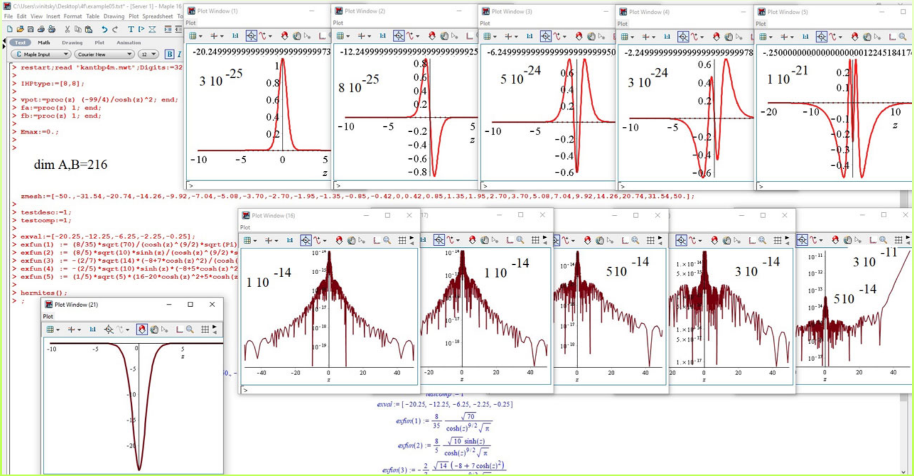
1D Interpolation Hermite Polynomials: Analytical formula

$$\varphi_r^{\kappa}(z) = w_r(z) \sum_{\kappa'=0}^{\kappa_r^{\max}-1} a_r^{\kappa,\kappa'} (z - z_r)^{\kappa'},$$

$$a_r^{\kappa,\kappa'} = \begin{cases} 0, & \kappa' < \kappa, \\ 1/\kappa'!, & \kappa' = \kappa, \\ -\sum_{\kappa''=\kappa}^{\kappa'-1} \frac{1}{(\kappa'-\kappa'')!} g_r^{\kappa'-\kappa''}(z_r) a_r^{\kappa,\kappa''}, & \kappa' > \kappa. \end{cases}$$

Note that all degrees of interpolation Hermite polynomials $\varphi_r^{\kappa}(z)$ do not depend on κ and equal $p' = \sum_{r'=0}^{p} \kappa_r^{\max} - 1$.

In the case of the nodes of identical multiplicity $\kappa_r^{\max} = \kappa^{\max}$, $r = 0, \ldots, p$ the degree of the polynomials is equal to $p' = \kappa^{\max}(p+1) - 1$.



> restart;read "kantbp4m.mwt";Digits:=32
> IHPtype:=[8,8];
> vpot:=proc(z) (-99/4)/cosh(z)^2; end;
> fa:=proc(z) 1; end;
> fb:=proc(z) 1; end;
> Emax:=0.;
dim A,B=216
zmesh:=[-50.,-31.54,-20.74,-14.26,-9.92,-7.04,-5.08,-3.70,-2.70,-1.95,-1.35,-0.85,-0.42,0,0.42,0.85,1.35,1.95,2.70,3.70,5.08,7.04,9.92,14.26,20.74,31.54,50.];
> testdesc:=1;
> testcomp:=1;
> exval:=[-20.25,-12.25,-6.25,-2.25,-0.25];
> hermites();
Plot Window (1)
-20.249999999999999999999999973
3 10 -25
Plot Window (2)
-12.249999999999999999999999925
8 10 -25
Plot Window (3)
-6.2499999999999999999999999950
5 10 -24
Plot Window (4)
-2.2499999999999999999999999978
3 10 -24
Plot Window (5)
-.25000000000000000000001224518417
1 10 -21
Plot Window (16)
1 10 -14
1 10 -14
5 10 -14
3 10 -14
3 10 -11
5 10 -14
Plot Window (21)
exval := [−20.25, −12.25, −6.25, −2.25, −0.25]

The economical implementation, accepted in FEM:

1. The calculations are performed in the local coordinates z', in which the coordinates of the simplex vertices are the following: $\hat{z}'_j = (\hat{z}'_{j1}, ..., \hat{z}'_{jd})$, $\hat{z}'_{jk} = \delta_{jk}$

$$z_i = \hat{z}_{0i} + \sum_{j=1}^{d} J_{ij} z'_j, \quad z'_i = \sum_{j=1}^{d} (J^{-1})_{ij}(z_j - \hat{z}_{0j}), \quad J_{ij} = \hat{z}_{ji} - \hat{z}_{0i}, \quad i = 1, ..., d.$$

$$\frac{\partial}{\partial z'_i} = \sum_{j=1}^{d} J_{ji} \frac{\partial}{\partial z_j}, \quad \frac{\partial}{\partial z_i} = \sum_{j=1}^{d} (J^{-1})_{ji} \frac{\partial}{\partial z'_j}.$$

2. The calculation of FEM integrals is executed in the local coordinates.

$$\int_{\Delta_q} dz g_0(z) \varphi_r^{\kappa}(z) \varphi_{r'}^{\kappa''}(z) U(z) = \hat{J} \int_{\Delta} dz' g_0(z(z')) \varphi_r^{\kappa}(z') \varphi_{r'}^{\kappa''}(z') U(z(z')), \quad \hat{J} = \det(J_{ij}) > 0$$

$$\int_{\Delta_q} dz g_{s_1 s_2}(z) \frac{\partial \varphi_r^{\kappa}(z)}{\partial z_{s_1}} \frac{\partial \varphi_{r'}^{\kappa''}(z)}{\partial z_{s_2}} = \hat{J} \sum_{t_1, t_2 = 1}^{d} (J^{-1})_{t_1 s_1} (J^{-1})_{t_2 s_2} \int_{\Delta} dz' g_{s_1 s_2}(z(z')) \frac{\partial \varphi_r^{\kappa}(z')}{\partial z'_{t_1}} \frac{\partial \varphi_{r'}^{\kappa''}(z')}{\partial z'_{t_2}},$$

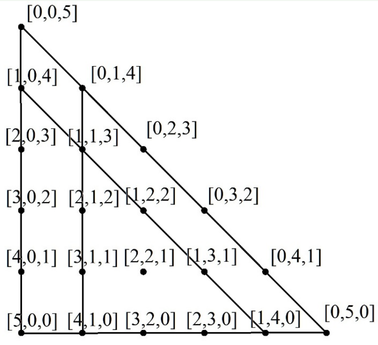
FEM calculation scheme

Each edge of the simplex Δ_q is divided into p equal parts and the families of parallel hyperplanes $H(i,k)$, $k=0,...,p$ are drawn. The equation of the hyperplane $H(i,k)$: $H(i;z)-k/p=0$, $H(i;z)$ is a linear on z.

The points A_r of hyperplanes crossingare enumerated with sets of hyperplane numbers: $[n_0,...,n_d]$, $n_i \geq 0$, $n_0+...+n_d=p$.

The coordinates $\xi_r=(\xi_{r1},...,\xi_{rd})$ of $A_r \in \Delta_q$:

$$\xi_r=\hat{z}_0 n_0/p+\hat{z}_1 n_1/p+...+\hat{z}_d n_d/p.$$



Lagrange Interpolation Polynomials (in the local coordinates)

$$\varphi_r(z')=\left(\prod_{i=1}^{d}\prod_{n'_i=0}^{n_i-1}\frac{z'_i-n'_i/p}{n_i/p-n'_i/p}\right)\left(\prod_{n'_0=0}^{n_0-1}\frac{1-z'_1-...-z'_d-n'_0/p}{n_0/p-n'_0/p}\right).$$

Algorithm for calculating the basis of Hermite interpolating polynomials

The problem

Constructions of the HIP of the order p', joining which the piecewise polynomial functions can be obtained that possess continuous derivatives to the given order κ'.

Step 1. Auxiliary polynomials (AP1)

$$\varphi_r^{\kappa_1\ldots\kappa_d}(\xi'_r)=\delta_{rr'}\delta_{\kappa_1 0}\ldots\delta_{\kappa_d 0}, \quad \left.\frac{\partial^{\mu_1+\ldots+\mu_d}\varphi_r^{\kappa_1\ldots\kappa_d}(z')}{\partial {z'_1}^{\mu_1}\ldots\partial {z'_d}^{\mu_d}}\right|_{z'=\xi'_{r'}}=\delta_{rr'}\delta_{\kappa_1\mu_1}\ldots\delta_{\kappa_d\mu_d},$$

$$0\leq\kappa_1+\kappa_2+\ldots+\kappa_d\leq\kappa_{\max}-1, \quad 0\leq\mu_1+\mu_2+\ldots+\mu_d\leq\kappa_{\max}-1.$$

Here in the node points ξ'_r, in contrast to LIP, the values of not only the functions themselves, but of their derivatives to the order $\kappa_{\max}-1$ are specified.

Algorithm for calculating the basis of Hermite interpolating polynomials

AP1 are given by the expressions

$$\varphi_r^{\kappa_1+\kappa_2+\ldots+\kappa_d}(z') = w_r(z') \sum_{\mu\in\Delta_\kappa} a_r^{\kappa_1\ldots\kappa_d,\mu_1\ldots\mu_d}(z'_1-\xi'_{r1})^{\mu_1}\times\ldots\times(z'_d-\xi'_{rd})^{\mu_d},$$

$$w_r(z') = \left(\prod_{i=1}^{d}\prod_{n'_i=0}^{n_i-1}\frac{(z'_i-n'_i/p)^{\kappa^{\max}}}{(n_i/p-n'_i/p)^{\kappa^{\max}}}\right)\left(\prod_{n'_0=0}^{n_0-1}\frac{(1-z'_1-\ldots-z'_d-n'_0/p)^{\kappa^{\max}}}{(n_0/p-n'_0/p)^{\kappa^{\max}}}\right),\quad w_r(\xi'_r)=1,$$

where the coefficients $a_r^{\kappa_1\ldots\kappa_d,\mu_1\ldots\mu_d}$ are calculated from recurrence relations

$$a_r^{\kappa_1\ldots\kappa_d,\mu_1\ldots\mu_d} = \begin{cases} 0, \quad \mu_1+\ldots+\mu_d\le\kappa_1+\ldots+\kappa_d, (\mu_1,\ldots,\mu_d)\ne(\kappa_1,\ldots,\kappa_d), \\ \prod_{i=1}^{d}\frac{1}{\mu_i!}, \qquad (\mu_1,\ldots,\mu_d)=(\kappa_1,\ldots,\kappa_d); \\ -\sum_{\nu\in\Delta_\nu}\left(\prod_{i=1}^{d}\frac{1}{(\mu_i-\nu_i)!}\right) g_r^{\mu_1-\nu_1,\ldots,\mu_d-\nu_d}(\xi'_r)\, a_r^{\kappa_1\ldots\kappa_d,\nu_1\ldots\nu_d}, \\ \qquad \mu_1+\ldots+\mu_d>\kappa_1+\ldots+\kappa_d; \end{cases}$$

$$g^{\kappa_1\kappa_2\ldots\kappa_d}(z') = \frac{1}{w_r(z')}\frac{\partial^{\kappa_1+\kappa_2+\ldots+\kappa_d}w_r(z')}{\partial {z'_1}^{\kappa_1}\partial {z'_2}^{\kappa_2}\ldots\partial {z'_d}^{\kappa_d}}.$$

Algorithm for calculating the basis of Hermite interpolating polynomials

For $d > 1$ and $\kappa_{\max} > 1$, the number $N_{\kappa_{\max}p'}$ of HIP of the order p' and the multiplicity of nodes $\kappa_{\max}$ are smaller than the number $N_{1p'}$ of the polynomials that form the basis in the space of polynomials of the order p', i.e., these polynomials, are determined ambiguously.

Step 2. Auxiliary polynomials (AP2 and AP3)

For unambiguous determination of the polynomial basis let us introduce $K = N_{1p'} - N_{\kappa_{\max}p'}$ auxiliary polynomials $Q_s(z)$ of two types: AP2 and AP3, linear independent of AP1 and satisfying the conditions in the node points $\xi'_{r'}$ of AP1:

$$Q_s(\xi'_{r'})=0, \quad \left.\frac{\partial^{\kappa'_1+\kappa'_2+\ldots+\kappa'_d} Q_s(z')}{\partial {z'_1}^{\mu_1}\partial {z'_2}^{\mu_2}\ldots\partial {z'_d}^{\mu_d}}\right|_{z'=\xi'_{r'}}=0, \quad s=1,\ldots,K,$$

$$0 \le \kappa_1+\kappa_2+\ldots+\kappa_d \le \kappa_{\max}-1, \quad 0 \le \mu_1+\mu_2+\ldots+\mu_d \le \kappa_{\max}-1.$$

AP2 for cont. of derivs. ($\eta'_{s'}$ on bounds of Δ):

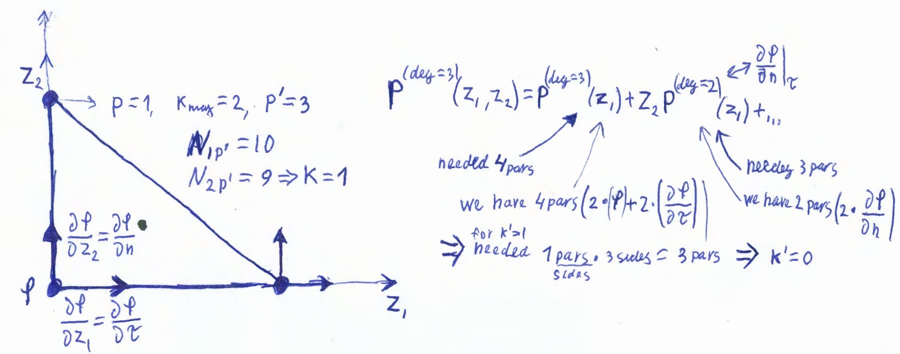
$$\left.\frac{\partial^k Q_s(z')}{\partial n^k_{i(s)}}\right|_{z'=\eta'_{s'}}=\delta_{ss'}, \quad s,s'=1,\ldots,T_1(\kappa').$$

AP3 ($\zeta'_{s'}$ inside Δ):

$$Q_s(\zeta'_{s'})=\delta_{ss'}, \quad s,s'=T_1(\kappa')+1,\ldots,K.$$

Construction of AP2 and AP3 at $d = 2$

Example 1: $p = 1$, $\kappa_{\max} = 2$, $p' = 3$, $\Rightarrow \kappa' = 0$

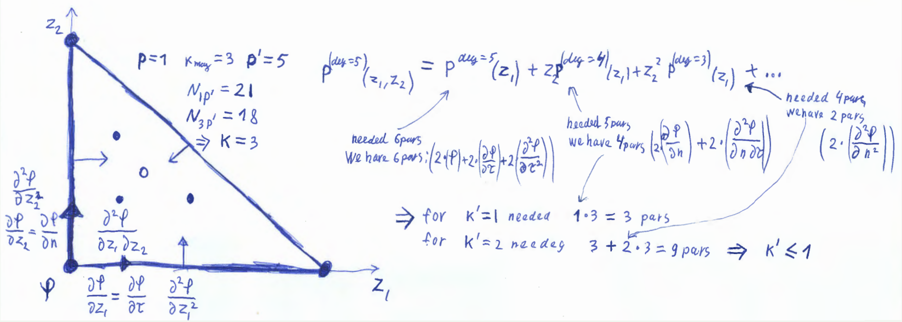


Alt. variant (Zienkievicz triangle)[a]: $\varphi(1/3, 1/3) = 0$

[a] Ciarlet, P.: The Finite Element Method for Elliptic Problems. North-Holland Publ. Comp, Amsterdam (1978)

Construction of AP2 and AP3 at $d = 2$

Example: $p = 1$, $\kappa_{\max} = 3$, $p' = 5$, $\Rightarrow \kappa' = 1$ (the Argyris triangle)



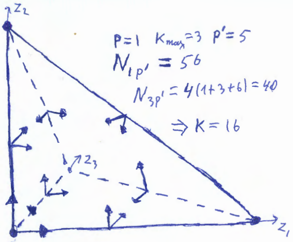
Argyris triangle ($\kappa' = 1$): AP1 (18 elements) + AP2 (3 elements: $\left.\frac{\partial^k Q_s(z')}{\partial n^k_{i(s)}}\right|_{z'=\eta'_{s'}} = \delta_{ss'}$ at $\eta'_{s'} \in \{(0, 1/2), (1/2, 0), (1/2, 1/2)\}$).

Alt. variant (Bell triangle, $\kappa' = 1$): $z_2 P^{\text{deg}=4}(z_1) \to z_2 P^{\text{deg}=3}(z_1)$, $\Leftrightarrow \left.\frac{\partial^5 \varphi(z')}{\partial n \partial \tau^4}\right|_{\delta\Delta} = 0$.

Alt. variant ($\kappa' = 0$): AP1 (18 elements) + AP3 (3 elements: $Q_s(\zeta'_{s'}) = \delta_{ss'}$ at $\eta'_{s'} \in \{(1/2, 1/4), (1/4, 1/2), (1/4, 1/4)\}$ or (Q_s or $\frac{\partial Q_s}{\partial z_1}$ or $\frac{\partial Q_s}{\partial z_2}$) $= \delta_{ss'}$ at $\eta'_{s'} \in (1/3, 1/3)$).

Construction of AP2 and AP3

Example 3 ($d = 3$): $p = 1$, $\kappa_{\max} = 3$, $p' = 5$, $\Rightarrow \kappa' = 0$



deg P(inside) = deg P(face) = deg P(rib); on a face we use IHP [131] ($d=2$)

$\Rightarrow \kappa' \leq 1$, and we have $\kappa_2 = \kappa - 4 \cdot N(AP2(d=2)) = 16 - 4\cdot 3 = \boxed{4 \text{(pars)}}$

rib: $p^{(deg=5)}(z_1 z_2 z_3) = p^{(deg=5)}(z_1) + z_2\, p^{(deg=4)}(z_1) + z_3\, p^{(deg=4)}(z_1) + \ldots$

(completed)

face: $p^{(deg=5)}(z_1 z_2 z_3) = p^{(deg=5)}(z_1 z_2) + z_3\, p^{(deg=4)}(z_1 z_2)$

(completed) needed 15 pars.

we have $3\cdot 3 + 3 \cdot 1 = 12$ $\left(\frac{\partial \varphi}{\partial z_3}\ \frac{\partial \varphi}{\partial z_3 \partial z_1}\ \frac{\partial \varphi}{\partial z_3 \partial z_2}\right)$

$\Rightarrow$ for $\kappa'=1$ needed $4\cdot(15-12) = 12 > 4$

$\Rightarrow \kappa' = 0$

So, at $d = 3$, $\kappa' = 1$ at $p' \geq 9$.

Simplest d-dimensional HIPs

Here $z_0 = 1 - z_1 - ... - z_d$, $i_k \neq i_l$, $i_k = 0, ..., d$

$p = 1$, $\kappa_{\max} = 2$, $p' = 3$

AP3: by 1 on each 2-faces[a]

$$z_{i_1} = z_{i_2} = z_{i_3} = 1/3, \quad Q_s(z) = 27 z_{i_1} z_{i_2} z_{i_3}$$

[a] Ciarlet, P.: The Finite Element Method for Elliptic Problems. North-Holland Publ. Comp, Amsterdam (1978)

$p = 1$, $\kappa_{\max} = 3$, $p' = 5$

AP3: by 3 on each 2-faces $z_{i_1} = z_{i_2} = 1/4, z_{i_3} = 1/2$,

$$Q_s(z) = -\frac{256}{25} z_{i_1} z_{i_2} z_{i_3} (5z_{i_1}^2 + 5z_{i_2}^2 - 45z_{i_3}^2 + 40 z_{i_1} z_{i_2} - 60 z_{i_1} z_{i_3} - 60 z_{i_2} z_{i_3} + z_{i_1} + z_{i_2} + 51 z_{i_3} - 6)$$

by 4 on each 3-faces $z_{i_1} = z_{i_2} = z_{i_3} = 1/5, z_{i_4} = 2/5$

$$Q_s(z) = -\frac{625}{2} z_{i_1} z_{i_2} z_{i_3} z_{i_4} (5 z_{i_4} - 1)$$

by 1 on each 4-faces $z_{i_1} = z_{i_2} = z_{i_3} = z_{i_4} = z_{i_5} = 1/5$

$$Q_s(z) = 3125 z_{i_1} z_{i_2} z_{i_3} z_{i_4} z_{i_5}$$

Simplest d-dimensional HIPs

$p = 1$, $\kappa_{\max} = 3$, $p' = 5$ (preserving first derivative iv vicinity of the edges)

AP2: by $d - 1$ derivatives in directions normal to the edge, at the center of edge.
Example

$$\left.\frac{\partial Q_2(z)}{\partial z_2}\right|_{z_1=1/2, z_2=\ldots=z_d=0} = 1$$

$$Q_2(z) = 8z_0 z_1 z_2 (2z_0 z_1 + (1 - z_0 - z_1 - z_2)(6/5 - 3z_0 - 3z_1 - z_2))$$

AP3: by 4 on each 3-faces $z_{i_1} = z_{i_2} = z_{i_3} = 1/5, z_{i_4} = 2/5$

$$Q_s(z) = -\frac{625}{2} z_{i_1} z_{i_2} z_{i_3} z_{i_4} (5z_{i_4} - 1)$$

by 1 on each 4-faces $z_{i_1} = z_{i_2} = z_{i_3} = z_{i_4} = z_{i_5} = 1/5$

$$Q_s(z) = 3125 z_{i_1} z_{i_2} z_{i_3} z_{i_4} z_{i_5}$$

The auxiliary polynomials AP2 and AP3:

$$Q_s(z') = {z'_1}^{k_1} ... {z'_d}^{k_d} (1 - z'_1 - ... - z'_d)^{k_0} \sum_{j_1,\dots,j_d} b_{j_1,\dots,j_d;s} {z'_1}^{j_1} ... {z'_d}^{j_d},$$

where $k_t = 1$, if the point η_s, in which the additional conditions are specified, lies on the corresponding face of the simplex Δ and $k_t = \max(1, \kappa')$, if $H(t, \eta_s) \neq 0$.
The coefficients $b_{j_1,\dots,j_d;s}$ are determined from the unambiguously solvable system of linear equations, obtained as a result of the substitution of this expression into the above conditions of Step 2.

Step 3: Recalculation of AP1

$$\check{\varphi}^{\kappa}_r(z') = \varphi^{\kappa}_r(z') - \sum_{s=1}^{K} c_{\kappa;r;s} Q_s(z'), \ \ c_{\kappa;r;s} = \begin{cases} \left. \dfrac{\partial^k \varphi^{\kappa}_r(z')}{\partial n^k_{i(s)}} \right|_{z'=\eta'_s}, & Q_s(z') \in \mathrm{AP2}, \\ \varphi^{\kappa}_r(\zeta_s), & Q_s(z') \in \mathrm{AP3}. \end{cases}$$

Step 4. Recalculation of AP1 and AP2 due to coordinate transformation

$$\frac{\partial}{\partial z_i} = \sum_{j=1}^{d} (\hat{J}^{-1})_{ji} \frac{\partial}{\partial z'_j}.$$

INTERNATIONAL JOURNAL FOR NUMERICAL METHODS IN ENGINEERING
Int. J. Numer. Meth. Engng 2005; **63**:455–471
Published online 3 March 2005 in Wiley InterScience (www.interscience.wiley.com). DOI: 10.1002/nme.1296

Tricubic interpolation in three dimensions

F. Lekien[*,†,1,2] and J. Marsden[2]

[1]*Mechanical and Aerospace Engineering, Princeton University, U.S.A.*
[2]*Control and Dynamical Systems, California Institute of Technology, U.S.A.*

SUMMARY

The purpose of this paper is to give a local tricubic interpolation scheme in three dimensions that is both C^1 and isotropic. The algorithm is based on a specific 64×64 matrix that gives the relationship between the derivatives at the corners of the elements and the coefficients of the tricubic interpolant for this element. In contrast with global interpolation where the interpolated function usually depends on the whole data set, our tricubic local interpolation only uses data in a neighbourhood of an element. We show that the resulting interpolated function and its three first derivatives are continuous if one uses cubic interpolants. The implementation of the interpolator can be downloaded as a static and dynamic library for most platforms. The major difference between this work and current local interpolation schemes is that we do not separate the problem into three one-dimensional problems. This allows for a much easier and accurate computation of higher derivatives of the extrapolated field. Applications to the computation of Lagrangian coherent structures in ocean data are briefly discussed.

KEY WORDS: tricubic; interpolation; computational dynamics

1. INTRODUCTION

1.1. Motivation from ocean dynamics

There has been considerable interest in using observational and model data available in coastal regions to compute Lagrangian structures such as barriers to transport and alleyways in the flow. As an example, Figure 1 shows the Lyapunov exponent field computed using high-frequency radar data collected in the bay of Monterey, along the California shoreline. Red denotes zones of higher stretching in the sense of Reference [1]. The bright red lines in Figure 1 define a boundary between the open ocean and a re-circulating area inside the bay. These

*Correspondence to: F. Lekien, E-Quad J220, Princeton University, Princeton, NJ 08544, U.S.A.
†E-mail: lekien@princeton.edu

Contract/grant sponsor: Office of Naval Research; contract/grant number: N00014-01-1-0208
Contract/grant sponsor: Office of Naval Research; contract/grant number: N00014-02-1-0826

Received 13 May 2004
Revised 23 August 2004
Accepted 13 December 2004

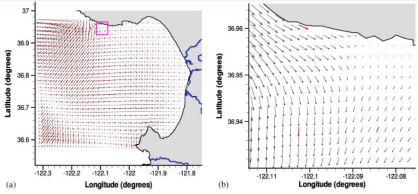


Figure 4. Experimentally observed velocity vectors (red arrows) in Monterey Bay, CA (see Reference [11] for details) and sampled velocity vectors (black arrows) resulting from the tricubic interpolation of the experimental data. Panel (a) shows the whole bay and panel (b) enlarges a small portion of the domain close to the coastline where a Dirichlet boundary condition has been properly enforced.

11. Paduan JD, Cook MS. Mapping surface currents in Monterey Bay with radar-type HR data. Oceanography 1997; 10:49–52.

IHP of d variables: extension of Lekien&Marsden's Algorithm

The IHPs of d variables in d-dimensional cube are calculated in analytical form as an product of one dimensional IHPs depending on each of the d variables

$$\varphi^{\kappa_1\ldots\kappa_d}_{i_1\ldots i_d}(x_1,\ldots,x_d)=\prod_{s=1}^{d}\varphi^{\kappa_s}_{i_s}(x_s),\quad \frac{\partial^{\kappa'_1+\ldots+\kappa'_d}\varphi^{\kappa_1\ldots\kappa_d}_{i_1\ldots i_d}}{\partial x_1^{\kappa'_1}\ldots x_d^{\kappa'_d}}(x'_1,\ldots,x'_d)=\delta_{x_1x'_1}\ldots\delta_{x_dx'_d}\delta_{\kappa_1\kappa'_1}\ldots\delta_{\kappa_d\kappa'_d},$$

where $\varphi^{\kappa_s}_{i_s}(x_s)$ are 1D IHPs.

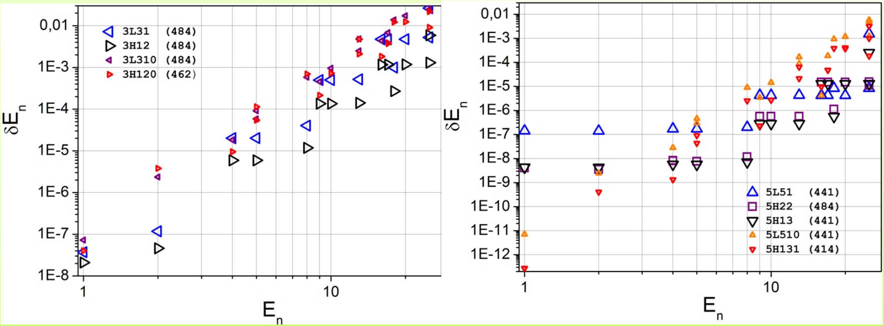
In particular, for $p=1$, $\kappa_{\max}=2$, $p'=3$ the one-dimensional IHPs take the form:

$$\varphi^{\kappa_s=0}_{i_s=0}(x_s)=(1-x_s)^2(1+2x_s),\quad \varphi^{\kappa_s=0}_{i_s=1}(x_s)=x_s^2(3-2x_s),$$

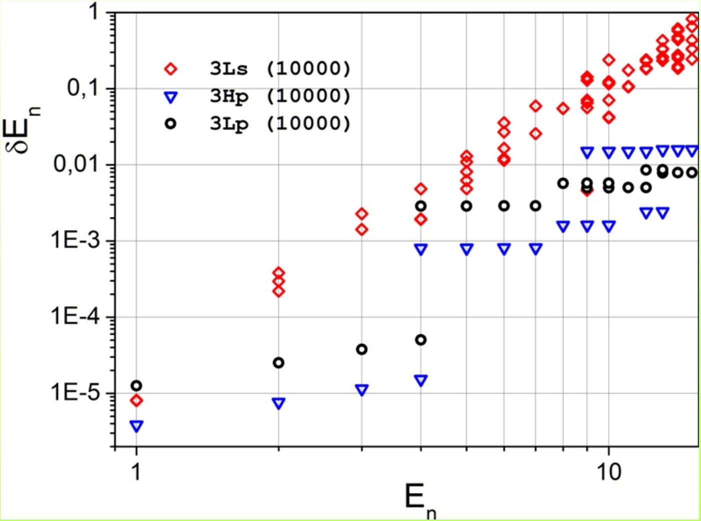
for polynomials whose value is equal to 1 at one node and

$$\varphi^{\kappa_s=1}_{i_s=0}(x_s)=(1-x_s)^2x_s,\quad \varphi^{\kappa_s=1}_{i_s=1}(x_s)=-x_s^2(1-x_s),$$

for polynomials whose first derivative is equal to 1 at one node.



The discrepancy $\delta E_m = E_m^h - E_m$ of calculated eigenvalue E_m^h of the Helmholtz problem for a square with the edge length π. Calculations were performed using FEM with 3rd-order and 5th-order (3Ls and 5Ls) simplex Lagrange elements, and parallelepiped Lagrange (3Lp and 5Lp) and Hermite (3Hp and 5Hp) elements. The dimension of the algebraic problem is given in parentheses.



The discrepancy $\delta E_m = E_m^h - E_m$ of calculated eigenvalue E_m^h of the Helmholtz problem for a four-dimensional cube with the edge length π. Calculations were performed using FEM with 3rd-order (3Ls) simplex Lagrange elements, and parallelepiped Lagrange (3Lp) and Hermite (3Hp) elements. The dimension of the algebraic problem is given in parentheses.

Resume

- The algorithms for constructing the multivariate interpolation Hermite polynomials in an analytical form in multidimensional hypercube or simplex are presented.
- Interpolation Hermite polynomials are determined from a specially constructed set of values of the polynomials themselves and their partial derivatives.
- The algorithms based on ideas of papers [a1—a5] allows us to avoid explicit solving the system of algebraic equations or reduce it.

a1 F. Lekien and J. Marsden, International Journal for Numerical Methods in Engineering, 63 (2005) 455–471.
a2 A. A. Gusev, et al., Lecture Notes in Computer Science, 8660 (2014) 138–154.
a3 A. A. Gusev, et al., Lecture Notes in Computer Science, 10490 (2017) 134–150.
a4 A. A. Gusev, et al., EPJ Web of Conferences, 173 (2018) 03009.
a5 A. A. Gusev, et al., EPJ Web of Conferences, 173 (2018) 03010.

Thank you for your attention