Arch. Rational Mech. Anal. 155 (2000) 215–235
Digital Object Identifier (DOI) 10.1007/s002050000111

Second-Order Structured Deformations

David R. Owen & Roberto Paroni

Abstract

Structured deformations provide a multi-scale geometrical setting for resolving the fields occurring in continuum mechanics into two parts: the part arising from smooth changes at smaller lengths scales and the part due to slips and separations (disarrangements) at smaller length scales. The portion without disarrangements is known to be associated with limits of gradients of approximating deformations, and the portion due to disarrangements corresponds to the effects of jumps in the approximating deformations. This paper extends the principal concepts and results on structured deformations to include the effects of limits of second gradients and jumps in the first gradients of approximating deformations and provides examples illustrating these effects. The resulting second-order structured deformations provide a setting for a complete description of structured motions and for the systematic treatment of mesolevel phase transitions, including the effects of jumps in first gradients on the bulk density of the Helmholtz free energy.

1. Introduction

Recent research on geometrical changes that can occur at different length scales has led to the concept of a structured deformation (κ, g, G) (see [1]). Here, the piecewise C^1 field g describes the macroscopic changes in the geometry of a continuous body, G is a piecewise continuous tensor field satisfying the inequality $\det G(x) \leqq \det \nabla g(x)$ at each point x, and κ is a surface-like subset of the body at which g and ∇g can have jump discontinuities. The main mathematical result in the theory of structured deformations is the Approximation Theorem [1]: *for each structured deformation, there exists a sequence $m \mapsto (\kappa_m,\ f_m)$ of "simple deformations", with the deformation field f_m continuously differentiable away from the* *set* κ_m*, such that*

$$\kappa = \liminf_{m\to\infty} \kappa_m := \bigcup_{m=1}^{\infty} \bigcap_{j=m}^{\infty} \kappa_j, \tag{1}$$

$$g = \lim_{m\to\infty} f_m, \tag{2}$$

$$G = \lim_{m\to\infty} \nabla f_m, \tag{3}$$

with the limits taken in the sense of (*essential*) *uniform convergence, i.e.,* L^∞ *convergence*. The sequence of simple deformations in the Approximation Theorem is called a *determining sequence* for the structured deformation (κ, g, G), and each term in the sequence (κ_m, f_m) is interpreted as revealing detailed geometrical changes, such as separation and slip on internal surfaces and smooth deformation away from these surfaces, not revealed by the macroscopic deformation $g = \lim_{m\to\infty} f_m$ alone. Moreover, incorporating $G = \lim_{m\to\infty} \nabla f_m$ into the description of geometrical changes reveals some aspects of the more detailed geometrical changes associated with a determining sequence. An application of a Gauss-Green formula for structured deformations [2] permits the derivation of the following formulas that further identify the tensors $G(x)$ and $M(x) := \nabla g(x) - G(x)$:

$$G(x) = \lim_{r\to 0} \lim_{m\to\infty} \operatorname{vol}(\mathcal{B}(x,r))^{-1} \int_{\mathcal{B}(x,r)\setminus\kappa_n} \nabla f_m(y) dV_y \tag{4}$$

$$M(x) = \lim_{r\to 0} \lim_{m\to\infty} \operatorname{vol}(\mathcal{B}(x,r))^{-1} \int_{\Gamma(f_m)\cap\mathcal{B}(x,r)} [f_m](y) \otimes \nu(y)\, dA_y. \tag{5}$$

The surface integral in the last relation is taken over the set $\Gamma(f_m)$ of jump points of f_m that lie inside the ball $\mathcal{B}(x,r)$ centered at x of radius r; the symbols $[f_m](y)$ and $\nu(y)$ in the surface integral are the jump in f_m at the point y and the normal to $\Gamma(f_m)$ at y, respectively. In view of the derived "identification relations" (4) and (5) for G and M, the formula

$$\nabla g(x) = G(x) + M(x) \tag{6}$$

represents an additive decomposition of the macroscopic deformation $\nabla g(x)$ into a *deformation without disarrangements* $G(x)$, associated with smooth geometrical changes at a smaller length scale, and a *deformation due to disarrangements* $M(x)$, associated with non-smooth changes at a smaller length scale. The familiar formula defining the gradient as a linear approximation, $g(y) - g(x) = \nabla g(x)(y-x) + o(y-x)$, and the additive decomposition (6) then yield the *refined linear approximation*

$$g(y) - g(x) = G(x)(y-x) + M(x)(y-x) + o(y-x) \tag{7}$$

in which the vector from $g(x)$ to $g(y)$, i.e., the translation from $g(x)$ to $g(y)$ in the deformed body, is decomposed to within terms $o(y-x)$ into a sum of the vector

$G(x)(y-x)$, the *translation without disarrangements*, and the vector $M(x)(y-x)$, the *translation due to disarrangements*.

Structured deformations have been applied to describe geometrical changes associated with slips and the presence of defects in single crystals, with deformations of liquid crystals, with fracture, and with the mixing of different substances [1,5, 7]. One limitation of structured deformations, as defined above, is that the effects on macroscopic deformation of jumps in the gradients ∇f_m of approximating simple deformations are not captured by the refined linear approximation (7). Another limitation is that the manner in which the quadratic approximation

$$g(y) - g(x) = \nabla g(x)(y - x) + \tfrac{1}{2}\nabla^2 g(x)[y - x, y - x] + o(|y - x|^2) \qquad (8)$$

should be refined to include the effects of deformations at smaller length scales is not revealed by structured deformations of the form (κ, g, G). (The second term on the right-hand side of (8) denotes the action of the bilinear mapping $\nabla^2 g(x)$ on the pair of vectors $[y - x, y - x]$.) Finally, definitive refinements of kinematical quantities such as acceleration and stretching are not available through such structured deformations. (See [5], however, for results on the refinement of velocity based on "space-time" structured deformations.)

Our goal in this paper is to provide a notion of "second-order structured deformation" (κ, g, G, Σ) that extends the scope of the multiscale geometry afforded by structured deformations of the original form (κ, g, G). (It is convenient from now on to distinguish the original structured deformations (κ, g, G) through the term "first-order structured deformations".) In Section 2 we adapt the notions of classical, simple, and structured deformations as defined in [1] in the first-order case to yield corresponding concepts for the second-order case. In particular, the additional entry Σ that appears in the symbol (κ, g, G, Σ) for a second-order structured deformation is a piecewise continuous, third-order tensor field possessing the same symmetries as a second gradient, but not being necessarily a second gradient itself. The remaining entries form a triple (κ, g, G) that turns out to be a first-order structured deformation in which g is piecewise twice continuously differentiable and G is piecewise continuously differentiable. Section 2 also contains a brief discussion of compositions of second-order structured deformations.

The principal results of this paper, the Approximation Lemma (Lemma 1) and the Approximation Theorem for second-order structured deformations (Theorem 2), are established in Section 3. The main difficulties in the analysis of second-order structured deformations are the necessity of constructing extensions of certain quadratic maps to the entire space as C^2 diffeomorphisms and the necessity of constructing injective mappings starting from a family of restrictions of the constructed C^2 diffeomorphisms. We overcome these difficulties in the proofs of Theorem 1 and the Approximation Lemma (Lemma 1). The remaining steps in establishing the results in Section 3 follow closely the analysis of the Approximation Lemma and the Approximation Theorem for first-order structured deformations [1]. In Section 4 we establish decompositions and identification relations that lead to the refinement of the basic quadratic approximation for macroscopic deformation (8). These results show how smooth deformations at smaller length scale, as well as jumps in deformation and in deformation gradient at a smaller length scale, contribute to the linear and quadratic terms in (8), yielding the desired refinement (48). An elementary example of second-order structured deformations is given in Section 3, and Section 5 is devoted to additional examples, including the bending of a rectangular block through distortions at smaller length scales without slips ("bending through simple shears"), and the bending of a block through distortions *and* slips at smaller length scales ("bending of a deck of cards").

A study of the energetics of first-order structured deformations has led to a more general setting for defining and analyzing structured deformations [6, 7], and a corresponding energetic analysis and extension for second-order structured deformations is in progress [8–10].

Notation and terminology. For each positive integer N, we let $\mathbb{R}^N$ denote the set of all N-tuples of real numbers $a = (a_1, \dots, a_N) = \big(a_p \in \mathbb{R} : p = 1, \cdots, N\big)$, we write $\mathbb{M}^{N\times N}$ for the set of all $N \times N$ real matrices

$$A = \big(A_{pq} \in \mathbb{R} \;:\; p, q = 1, \cdots, N\big),$$

and we denote by $\mathbb{M}^{N\times N\times N}$ the set of all real arrays

$$\Xi = \big(\Xi_{pqr} \in \mathbb{R} \;:\; p, q, r = 1, \cdots, N\big).$$

Of course, the matrices $A \in \mathbb{M}^{N\times N}$ are put in one-to-one correspondence with the linear mappings $L \in \mathrm{Lin}(\mathbb{R}^N)$ by means of the mapping:

$$A \mapsto L_A := a \mapsto \left(\sum_{q=1}^{N} A_{pq} a_q \;:\; p = 1, \cdots, N\right) = Aa,$$

and we define norms on $\mathbb{R}^N$ and $\mathbb{M}^{N\times N}$ through the formulas

$$\|a\| := \left(\sum_{i=1}^{N} a_i^2\right)^{\frac{1}{2}}, \tag{9}$$

$$\|A\| := \sup_{a\neq 0} \frac{\|Aa\|}{\|a\|}, \tag{10}$$

respectively.

The arrays $\Xi \in \mathbb{M}^{N\times N\times N}$ are put in one-to-one correspondence with the bilinear mappings $B \in \mathrm{Lin}_2(\mathbb{R}^N, \mathbb{R}^N)$ through the mapping

$$\Xi \mapsto B_\Xi := (a, b) \mapsto \left(\sum_{q,r=1}^{N} \Xi_{pqr} a_q b_r \;:\; p = 1, \cdots, N\right) =: \Xi[a, b];$$

Ξ (or B_Ξ) is said to be *symmetric* if $\Xi[a, b] = \Xi[b, a]$ for all $a, b \in \mathbb{R}^N$. (Equivalently, Ξ is symmetric if $\Xi_{pqr} = \Xi_{prq}$ for all $p, q, r = 1, \cdots, N$.) Moreover, each $a \in \mathbb{R}^N$ and $\Xi \in \mathbb{M}^{N\times N\times N}$, determine a linear mapping $L_{\Xi,a} \in \mathrm{Lin}\,\mathbb{R}^N$ through the formula $L_{\Xi,a} := \Xi[a, \cdot]$, i.e.,

$$L_{\Xi,a}\, b := \Xi[a, b] \quad \text{for all } b \in \mathbb{R}^N,$$

and the formula

$$\|\Xi\| := \sup_{a\neq 0, b\neq 0} \frac{\|\Xi[a,b]\|}{\|a\|\|b\|} = \sup_{a\neq 0} \frac{\|\Xi[a,\cdot]\|}{\|a\|} \tag{11}$$

defines a norm on $\mathbb{M}^{N\times N\times N}$. If $A \in \mathbb{M}^{N\times N}$ and $p, q = 1, \cdots, N$, then A_{pq} denotes the p-q-th component of L_A with respect to the standard basis on $\mathbb{R}^N$, and we have $\left|A_{pq}\right| \leqq \|A\|$. For each $p = 1, \cdots, N$, we denote by $I_p(A)$ the p-th invariant of A, i.e., the sum of the determinants of all of the principal $p \times p$ submatrices of A (see the proof of Proposition 2 in Section 3). The symbol I alone denotes the $N \times N$ identity matrix $I = \mathrm{diag}(1, 1, \cdots, 1)$, and $\mathcal{B}(x, r)$ denotes the open ball centered at $x \in \mathbb{R}^N$ of radius $r > 0$.

For each subset $\mathcal{A}$ of $\mathbb{R}^N$, we denote by $\overline{\mathcal{A}}$ the closure of $\mathcal{A}$, by $\partial\mathcal{A}$ the boundary of $\mathcal{A}$, and by $\mathcal{A}^\circ$ the interior of $\mathcal{A}$. A C^2 *diffeomorphism* of $\mathbb{R}^N$ is a bijective, C^2 mapping $f : \mathbb{R}^N \to \mathbb{R}^N$ whose inverse also is of class C^2.

2. Definitions and preliminaries

The regions that a deforming body can occupy are described here in terms of "fit regions" [3]: a fit region of $\mathbb{R}^N$ is a bounded, regularly open set with finite perimeter whose boundary has measure zero. As is the case for first-order structured deformations, the notion of a second-order structured deformation is based on notions of "classical deformations" and "simple deformations", defined here simply by strengthening the smoothness requirements on mappings from "C^1", in the first-order case [1], to "C^2" in the present case.

Definition 1. Let $\mathcal{A}$ be a fit region in $\mathbb{R}^N$. A *classical deformation from* $\mathcal{A}$ is a mapping f from $\mathcal{A}$ into $\mathbb{R}^N$ satisfying:

(Cld 1) f can be extended to a C^2 diffeomorphism of $\mathbb{R}^N$;
(Cld 2) f is orientation preserving, i.e.,

$$\det\nabla f(x) > 0 \text{ for all } x \in \mathcal{A}.$$

We recall that a *piecewise fit region* [1] is a finite union of (possibly overlapping) fit regions.

Definition 2. Let $\mathcal{A}$ be a piecewise fit region in $\mathbb{R}^N$. A *simple deformation from* $\mathcal{A}$ is a pair (κ, f), where κ is a subset of $\mathcal{A}$ and f is mapping from $\mathcal{A} \setminus \kappa$ into $\mathbb{R}^N$, with the following properties:

(Sid 1) vol $\kappa = 0$;
(Sid 2) f is injective;
(Sid 3) $\mathcal{A} \setminus \kappa$ is the union of finitely many fit regions such that the restriction of f to each of the fit regions is a classical deformation.

Definition 3. Let $\mathcal{A}$ be a piecewise fit region in $\mathbb{R}^N$. A *second-order structured deformation from* $\mathcal{A}$ is a quadruple (κ, g, G, Σ) in which

(Std 1) (κ, g) is a simple deformation from $\mathcal{A}$;

(Std 2) $G : \mathcal{A} \setminus \kappa \to \mathrm{Lin}\,(\mathbb{R}^N)$ is of class C^1, $\Sigma : \mathcal{A} \setminus \kappa \to \mathrm{Lin}_2(\mathbb{R}^N, \mathbb{R}^N)$ is symmetric (i.e., for every $x \in \mathcal{A} \setminus \kappa$, $\Sigma(x)$ is symmetric) and continuous, G has a piecewise C^1 extension to $\overline{\mathcal{A}}$, and Σ has a piecewise continuous extension to $\overline{\mathcal{A}}$, in the sense that there exists a finite collection of fit regions $\{\mathcal{A}_j : j = 1, \ldots, J\}$ whose union is $\mathcal{A} \setminus \kappa$ such that, for each $j = 1, \ldots, J$, $G|_{\mathcal{A}_j}$ has a C^1 extension to $\overline{\mathcal{A}_j}$ and $\Sigma|_{\mathcal{A}_j}$ has a continuous extension to $\overline{\mathcal{A}_j}$.

(Std 3) There exists $m > 0$ such that $m < \det G(x) \leqq \det \nabla g(x)$ for all $x \in \mathcal{A} \setminus \kappa$.

We note that the fields g, G, and Σ associated with a second-order structured deformation, as well as the fields f, ∇f, and $\nabla^2 f$ associated with a simple deformation, are bounded.

The next definition provides a precise sense in which one can assert that a sequence of simple deformations approaches a second-order structured deformation.

Definition 4. Let $\mathcal{A}$ be a piecewise fit region in $\mathbb{R}^N$. We say that the sequence $m \mapsto (\kappa_m, f_m)$ of simple deformations from $\mathcal{A}$ *determines* the second-order structured deformation (κ, g, G, Σ) from $\mathcal{A}$, if the following conditions are satisfied:

$$\kappa = \liminf_{m \to \infty} \kappa_m := \bigcup_{m=1}^{\infty} \bigcap_{j=m}^{\infty} \kappa_j, \tag{12}$$

$$\lim_{m \to \infty} \|g - f_m\|_{L^\infty(\mathcal{A}, \mathbb{R}^N)} = 0, \tag{13}$$

$$\lim_{m \to \infty} \|G - \nabla f_m\|_{L^\infty(\mathcal{A}, \mathrm{Lin}(\mathbb{R}^N, \mathbb{R}^N))} = 0, \tag{14}$$

$$\lim_{m \to \infty} \|\Sigma - \nabla^2 f_m\|_{L^\infty(\mathcal{A}, \mathrm{Lin}_2(\mathbb{R}^N, \mathbb{R}^N))} = 0. \tag{15}$$

Our final definition embodies the idea that a body may undergo a simple deformation followed by a second-order structured deformation.

Definition 5. Let (κ, f) be a simple deformation from $\mathcal{A}$, and let (μ, h, H, Θ) be a second-order structured deformation from $f(\mathcal{A} \setminus \kappa)$. Then the *composition* of (μ, h, H, Θ) with (κ, f) is the quadruple defined by

$$\begin{aligned}(\mu, h, H, \Theta) \circ (\kappa, f) = \Big(&\kappa \cup f^{-1}(\mu),\ h \circ f\ |_{\mathcal{A} \setminus (\kappa \cup f^{-1}(\mu))}, \\ &\big(H \circ f\ |_{\mathcal{A} \setminus (\kappa \cup f^{-1}(\mu))}\big) \nabla f\ |_{\mathcal{A} \setminus (\kappa \cup f^{-1}(\mu))}, \\ &\big(\Theta \circ f\ |_{\mathcal{A} \setminus (\kappa \cup f^{-1}(\mu))}\big)\big[\nabla f\ |_{\mathcal{A} \setminus (\kappa \cup f^{-1}(\mu))}, \nabla f\ |_{\mathcal{A} \setminus (\kappa \cup f^{-1}(\mu))}\big] \\ &+ \big(H \circ f\ |_{\mathcal{A} \setminus (\kappa \cup f^{-1}(\mu))}\big) \nabla^2 f\ |_{\mathcal{A} \setminus (\kappa \cup f^{-1}(\mu))}\Big).\end{aligned} \tag{16}$$

For each simple deformation (κ, f), the quadruple $(\kappa, f, \nabla f, \nabla^2 f)$ turns out to be a second-order structured deformation, and the formula (16) then leads to a concept of composition for pairs of second-order structured deformations in which the first need not arise from a simple deformation. (We shall not have need of this more general composition in the present development.)

It is a routine matter to verify that the composition $(\mu, h, H, \Theta) \circ (\kappa, f)$ is a second-order structured deformation from the piecewise fit region $\mathcal{A}$. Moreover, the next result shows that a determining sequence for (μ, h, H, Θ) yields immediately a determining sequence for $(\mu, h, H, \Theta) \circ (\kappa, f)$.

Proposition 1. *Let (κ, f) be a simple deformation from $\mathcal{A}$, and let (μ, h, H, Θ) be a second-order structured deformation from $f(\mathcal{A}\backslash\kappa)$. Let $m \mapsto (\mu_m, h_m)$ be a sequence of simple deformations from $f(\mathcal{A}\backslash\kappa)$ that determines (μ, h, H, Θ). Then the sequence of simple deformations*

$$m \mapsto (\mu_m, h_m) \circ (\kappa, f) := (\kappa \cup f^{-1}(\mu_m), h_m \circ f \,|_{\mathcal{A}\backslash(\kappa \cup f^{-1}(\mu_m))})$$

determines the second-order structured deformation $(\mu, h, H, \Theta) \circ (\kappa, f)$.

Proof. We notice that

$$\begin{aligned} &\|(\nabla^2 h_m \circ f)[\nabla f, \nabla f] + (\nabla h_m \circ f)\nabla^2 f \\ &\qquad - (\Theta \circ f)[\nabla f, \nabla f] - (H \circ f)\nabla^2 f\|_{L^\infty(\mathcal{A})} \\ &\qquad\qquad \leqq \|\nabla^2 h_m - \Theta\|_{L^\infty(\mathcal{A}\backslash\kappa)}\|\nabla f\|^2_{L^\infty(\mathcal{A})} \\ &\qquad\qquad\quad + \|\nabla h_m - H\|_{L^\infty(\mathcal{A}\backslash\kappa)}\|\nabla^2 f\|_{L^\infty(\mathcal{A})} \to 0 \end{aligned}$$

as $m \to \infty$. The rest of the proof is identical to the one given in [1], Proposition 4.9. □

3. Approximation theorem

In this section we shall establish the Approximation Theorem for second-order structured deformations (Theorem 2, below): every second-order structured deformation has a determining sequence. The existence of a determining sequence reveals, by means of relations (12)–(15), geometrical information about each entry in a second-order structured deformation (κ, g, G, Σ) that is not apparent from Definition 3 and that is useful in a variety of situations.

Our first result provides elementary estimates required for the proof of Theorem 1.

Proposition 2. *For each $A \in \mathbb{M}^{N\times N}$,*

$$1 - \sum_{j=1}^{N} j! \binom{N}{j} \|A\|^j \leqq \det(I + A) \leqq 1 + \sum_{j=1}^{N} j! \binom{N}{j} \|A\|^j. \tag{17}$$

If $B \in \mathbb{M}^{N\times N}$ is a symmetric matrix whose eigenvalues are less than or equal to 1 *in absolute value, then*

$$|I_j(AB)| \leqq j! \binom{N}{j} \|A\|^j \qquad \text{for every } j = 1, \ldots, N. \tag{18}$$

Proof. By induction it is easy to see that if $H \in M^{j\times j}$ then $|\det H| \leqq j!\|H\|^j$. To verify (18), let $\alpha \subset \{1, 2, \dots, N\}$ be an index set. For each matrix $E \in \mathbb{M}^{N\times N}$ we denote the submatrix that lies in the rows and columns of E indexed by α as $E(\alpha)$. If α has j elements then we write $\#(\alpha) = j$ and call the submatrix $E(\alpha)$ a principal submatrix of order j. Let us choose a basis of $\mathbb{R}^N$ such that $B = \operatorname{diag}(\beta_1, \cdots, \beta_N)$. It follows by multiplication of matrices, that $(AB)(\alpha) = A(\alpha)B(\alpha)$. Hence, since $|\det B(\alpha)| \leqq 1$,

$$|\det(AB)(\alpha)| = |\det A(\alpha)||\det B(\alpha)| \leqq |\det A(\alpha)|.$$

The definition of the principle invariant $I_j(AB)$ then yields

$$\begin{aligned} |I_j(AB)| &= \left|\sum_{\#(\alpha)=j} \det((AB)(\alpha))\right| \leqq \sum_{\#(\alpha)=j} |\det A(\alpha)| \leqq \sum_{\#(\alpha)=j} j!\|A\|^j \\ &= \binom{N}{j} j!\|A\|^j, \end{aligned}$$

where we have used the fact that there are $\binom{N}{j}$ different principal submatrices of order j, and this establishes (18). To complete the proof, we apply (18) with $B = I$ to obtain the inequality

$$\left|I_j(A)\right| \leqq \binom{N}{j} j!\|A\|^j,$$

and then we use the relation

$$\det(I + A) = 1 + \sum_{j=1}^{N} I_j(A)$$

together with the triangle inequality to obtain (17). □

The next result provides smooth diffeomorphic extensions to the entire space for members of a particular class of quadratic functions.

Theorem 1. *Let* $a \in \mathbb{R}^N$, $A \in \operatorname{Lin}(\mathbb{R}^N, \mathbb{R}^N)$, $\Xi \in \operatorname{Lin}_2(\mathbb{R}^N, \mathbb{R}^N)$, *and positive real numbers* m, M *be given such that* $m \leqq \det A < M$ *and* Ξ *is symmetric. There exists* $r = r(M, \det A, \|A^{-1}\Xi\|) > 0$ *depending continuously on* $(M, \det A, \|A^{-1}\Xi\|)$ *such that the function* $f : \mathcal{B}(0, r) \to \mathbb{R}^N$ *defined by*

$$f(x) = \tfrac{1}{2}\Xi[x, x] + Ax + a \tag{19}$$

can be extended to a C^2 *diffeomorphism* f^e *of* $\mathbb{R}^N$ *that satisfies*

$$\frac{m}{2} \leqq \det \nabla f^e(x) < M \tag{20}$$

for every $x \in \mathbb{R}^N$.

Proof. We put $\Lambda := A^{-1}\Xi$, i.e., $\Lambda_{ijk} = (A^{-1})_{ip}\Xi_{pjk}$ and choose $r_1 > 0$ such that

$$r_1 < \sup\left\{ q > 0 : \frac{M}{\det A} > 1 + \sum_{j=1}^{N} j! \binom{N}{j} \|\Lambda\|^j s^j \right.$$
$$\left. \text{and } 1 - \sum_{j=1}^{N} j! \binom{N}{j} \|\Lambda\|^j s^j > \frac{1}{2} \text{ for all } s \in [0, q] \right\}.$$

Further, we choose a number r_2 satisfying $0 < r_2 \leqq \min\left\{r_1, (7\|\Lambda\|)^{-1}\right\}$; for example, elementary estimates show that we may put

$$r_2 := \min\left\{ (7\|\Lambda\|)^{-1}, (N!(1+\|\Lambda\|)^N)^{-1}\frac{1}{2}, (N!(1+\|\Lambda\|)^N)^{-1}\frac{M - \det A}{\det A} \right\}. \tag{21}$$

We put $r := r_2/4$, and we choose a C^2 function $\psi : (0,\infty) \to \mathbb{R}$ satisfying $\psi = 1$ on $(0, r)$, $\psi = 0$ on (r_2, ∞) and $-2/r_2 \leqq \psi'(x) \leqq 0$ for every $x \in (0,\infty)$. We define $f^e : \mathbb{R}^N \to \mathbb{R}^N$ by

$$f^e(x) = \psi(\|x\|)\tfrac{1}{2}\Xi[x, x] + Ax + a,$$

and we notice that f^e is a C^2 extension of the function f defined in (19) from $\mathcal{B}(0, r)$ to $\mathbb{R}^N$. The gradient of f^e is

$$\begin{aligned}
\nabla f^e(x) &= \psi'(\|x\|)\frac{1}{2}\Xi[x, x] \otimes \frac{x}{\|x\|} + \psi(\|x\|)\Xi[x, \cdot] + A \\
&= A\left(\frac{1}{2}\psi'(\|x\|)\Lambda[x, x] \otimes \frac{x}{\|x\|} + \psi(\|x\|)\Lambda[x, \cdot] + I\right) \\
&= A\left(\Lambda[x, \cdot]\left(\frac{1}{2}\psi'(\|x\|)x \otimes \frac{x}{\|x\|} + \psi(\|x\|)I\right) + I\right) \\
&= A(\Lambda[x, \cdot]B(x) + I),
\end{aligned}$$

where the symmetric matrix $B(x)$ is defined by

$$B(x) = \frac{1}{2}\psi'(\|x\|)x \otimes \frac{x}{\|x\|} + \psi(\|x\|)I$$

and where $\otimes$ denotes the tensor product: $(c \otimes d)e = (d \cdot e)c$ for all $c, d, e \in \mathbb{R}^N$. We now show that the function f^e satisfies (20). For $\|x\| \geqq r_2$ we have $f^e(x) = Ax + a$ and hence (20) is clearly satisfied. For $\|x\| < r$ we have that $\psi(\|x\|) = 1$ and hence $B(x) = I$. By using (17) we obtain the relations

$$\begin{aligned}
\det \nabla f^e(x) &= \det A \det(I + \Lambda[x, \cdot]) \\
&\in \det A\left(1 - \sum_{j=1}^{N} j! \binom{N}{j} \|\Lambda[x, \cdot]\|^j, 1 + \sum_{j=1}^{N} j! \binom{N}{j} \|\Lambda[x, \cdot]\|\right) \\
&\subset \det A\left(1 - \sum_{j=1}^{N} j! \binom{N}{j} \|\Lambda\|^j \frac{r_2^j}{4^j}, 1 + \sum_{j=1}^{N} j! \binom{N}{j} \|\Lambda\|^j \frac{r_2^j}{4^j}\right),
\end{aligned}$$

and, in view of (21), (20) is satisfied since $r = r_2/4 \leqq r_1$. Finally, for $r \leqq \|x\| \leqq r_2$ we notice that the absolute value of each of the eigenvalues of $B(x)$ is less than 1. In fact, for each $\xi \in \mathbb{R}^N$ we have

$$B(x)\xi \cdot \xi = -\frac{1}{2}|\psi'(\|x\|)|\|x\| \left(\frac{x \cdot \xi}{\|x\|}\right)^2 + \psi(\|x\|)\|\xi\|^2;$$

hence

$$B(x)\xi \cdot \xi \leqq \psi(\|x\|)\|\xi\|^2 \leqq \|\xi\|^2,$$

and

$$B(x)\xi \cdot \xi \geqq -\frac{1}{2}|\psi'(\|x\|)|\|x\| \left(\frac{x \cdot \xi}{\|x\|}\right)^2 \geqq -\frac{1}{2}\frac{2}{r_2}\|x\|\|\xi\|^2 \geqq -\|\xi\|^2.$$

From this bound on the eigenvalues of $B(x)$, the last equation in the proof of Proposition 2 along with (18) and (17) yield

$$\begin{aligned}
\det \nabla f^e(x) &= \det A \det(I + \Lambda[x,\cdot]B(x)) \\
&\in \det A \left(1 - \sum_{j=1}^{N} |I_j(\Lambda[x,\cdot]B(x))|, 1 + \sum_{j=1}^{N} |I_j(\Lambda[x,\cdot]B(x))|\right) \\
&\subset \det A \left(1 - \sum_{j=1}^{N} j! \binom{N}{j} \|\Lambda[x,\cdot]\|^j, 1 + \sum_{j=1}^{N} j! \binom{N}{j} \|\Lambda[x,\cdot]\|^j\right) \\
&\subset \det A \left(1 - \sum_{j=1}^{N} j! \binom{N}{j} \|\Lambda\|^j r_2^j, 1 + \sum_{j=1}^{N} j! \binom{N}{j} \|\Lambda\|^j r_2^j\right),
\end{aligned}$$

and, keeping in mind that $r_2 \leqq r_1$, we conclude that (20) is satisfied.

We now show that f^e is injective. Since for $\|x\| > r_2$ the function $x \mapsto f^e(x)$ is injective, it suffices to consider the relation $f^e(x) = f^e(\tilde{x})$ when $\|x\| \leqq r_2$ and $\|\tilde{x}\|$ is unrestricted. If $\|x\| \leqq r_2$ and $\|\tilde{x}\| \geqq r_2$, then $f^e(x) = f^e(\tilde{x})$ implies $\tilde{x} = x + \frac{1}{2}\psi(\|x\|)\Lambda[x,x]$, so that

$$\|x - \tilde{x}\| \leqq \tfrac{1}{2}\|\Lambda\|\,\|x\|^2 \leqq \tfrac{1}{2}\|\Lambda\|\,r_2^2 \leqq r_2.$$

Therefore, when $\|x\| \leqq r_2$ and $\|\tilde{x}\| \geqq r_2$, $f^e(x) = f^e(\tilde{x})$ implies that $\|\tilde{x}\| \leqq 2r_2$. Thus, it suffices to establish the injectivity of $x \mapsto f^e(x)$ on $\overline{\mathcal{B}(0, 2r_2)}$, the closed ball of radius $2r_2$ centered at 0. Let $y \in \mathbb{R}^N$ be given and define $\xi(x) = x + A^{-1}(y - f^e(x))$ for each $x \in \mathbb{R}^N$. We note that $\xi(x) = x$ if and only if $f^e(x) = y$, so to prove the injectivity of f^e it suffices to show that ξ has at most one fixed point in $\overline{\mathcal{B}(0, 2r_2)}$. The Mean Value Theorem, the inequality $r_2 \leqq 1/(7\|\Lambda\|)$, and the estimate

$$\begin{aligned}
\|\nabla\xi(x)\| = \|I - A^{-1}\nabla f^e(x)\| &= \left\|\Lambda[x,\cdot]\left(\frac{1}{2}\psi'(\|x\|)x \otimes \frac{x}{\|x\|} + \psi(\|x\|)I\right)\right\| \\
&\leqq \|\Lambda\|\|x\|\left(\frac{1}{2}\frac{2}{r_2}\|x\| + 1\right) \leqq \|\Lambda\|2r_2(2+1) = 6r_2\|\Lambda\|
\end{aligned}$$

show that $\|\xi(x) - \xi(\tilde{x})\| < \|x - \tilde{x}\|$ for all $x, \tilde{x} \in \overline{\mathcal{B}(0, 2r_2)}$ with $x \neq \tilde{x}$. Hence ξ has at most one fixed point on that ball. Thus, f^e is an injective, C^2 function with $\det \nabla f^e > 0$, and the Inverse Function Theorem tell us that f^e is locally invertible with a local inverse that is of class C^2.

In order to show that $f^e : \mathbb{R}^N \to \mathbb{R}^N$ is a C^2 diffeomorphism, it remains to show that the range of f^e is equal to $\mathbb{R}^N$. Because $f^e(x) = Ax + a$ for all $x \in \mathbb{R}^N \backslash \mathcal{B}(0, r_2)$, the injectivity of f^e and the invertibility of $(x \mapsto Ax + a) : \mathbb{R}^N \to \mathbb{R}^N$ yield

$$f^e(\mathcal{B}(0, r_2)) \subset \mathcal{A}(r_2) := \{Ax + a : |x| < r_2\}$$

and

$$f^e(\mathbb{R}^N \backslash \mathcal{B}(0, r_2)) = \mathbb{R}^N \backslash \mathcal{A}(r_2).$$

However, the inclusion in the first relation above must be equality. In fact, suppose, to the contrary, that $f^e(\mathcal{B}(0, r_2)) \neq \mathcal{A}(r_2)$. Then we may choose $y \in \mathcal{A}(r_2) \backslash f^e(\mathcal{B}(0, r_2))$. If $y \in \partial f^e(\mathcal{B}(0, r_2))$ the continuity and injectivity of f^e imply that $y \in \partial f^e(\mathcal{B}(0, r_2)) = f^e(\partial \mathcal{B}(0, r_2))$, and therefore there exists an $\tilde{x} \in \partial \mathcal{B}(0, r_2)$ such that $f^e(\tilde{x}) = A\tilde{x} + a = y$. But this contradicts the fact that $y \in \mathcal{A}(r_2)$ and that $x \mapsto Ax + a$ is an injective mapping. Thus $y \notin \partial f^e(\mathcal{B}(0, r_2))$ and hence $f^e(\mathcal{B}(0, r_2))$ is closed in $\mathcal{A}(r_2)$, since we can find a small ball centered in y, open in $\mathcal{A}(r_2)$ and which does not intersect $\partial f^e(\mathcal{B}(0, r_2))$. On the other hand, the local invertibility of f^e implies that $f^e(\mathcal{B}(0, r_2))$ is open in $\mathcal{A}(r_2)$. However, $\mathcal{A}(r_2)$ is connected and $f^e(\mathcal{B}(0, r_2))$ is a non-empty open and closed subset of $\mathcal{A}(r_2)$, so $f^e(\mathcal{B}(0, r_2)) = \mathcal{A}(r_2)$, which contradicts our assumption. Thus $f^e(\mathcal{B}(0, r_2)) = \mathcal{A}(r_2)$,

$$f^e(\mathbb{R}^N) = f^e(\mathcal{B}(0, r_2)) \cup f^e(\mathbb{R}^N \backslash \mathcal{B}(0, r_2)) = \mathcal{A}(r_2) \cup \left(\mathbb{R}^N \backslash \mathcal{A}(r_2)\right) = \mathbb{R}^N,$$

and f^e is surjective. □

Example 1. Put $N := 1$, $\mathcal{A} := (0, 1)$, and, for each positive integer n and $i = 0, 1, \ldots, n$, put $x_i := i/n$ and $\kappa_n := \{x_i : i = 1, 2, \ldots, n-1\}$. Let $\Sigma \in \mathbb{R}$ be given, and define for each $x \in (0, 1) \backslash \kappa_n$

$$f_n(x) := \sum_{i=0}^{n-1} \left(x_i + (1 - |\Sigma|/n)(x - x_i) + \tfrac{1}{2}\Sigma(x - x_i)^2\right) \chi_{(x_i, x_{i+1})}(x), \qquad (22)$$

where $\chi_{(x_i, x_{i+1})}$denotes the characteristic function of the interval (x_i, x_{i+1}). To show that (κ_n, f_n) is a simple deformation, it suffices to show that f_n is injective and, for every $i = 0, 1, \ldots, n-1$, that f_n restricted to (x_i, x_{i+1}) is a classical deformation . Note that for $n > 2|\Sigma|$

$$f_n'(x) = \sum_{i=0}^{n-1} \left(1 - \frac{|\Sigma|}{n} + \Sigma(x - x_i)\right) \chi_{(x_i, x_{i+1})}(x) \geqq 1 - 2\frac{|\Sigma|}{n} > 0.$$

Thus, for n large enough, we are in position to apply Theorem 1 and, hence, to conclude that f_n restricted to (x_i, x_{i+1}) can be extended to a C^2 diffeomorphism of $\mathbb{R}$. We now show that f_n is injective. Since f_n is increasing on each interval (x_i, x_{i+1}) for n large enough, it suffices to check that

$$f_n(x_i^-) := \lim_{x \to x_i^-} f_n(x) \leqq \lim_{x \to x_i+} f_n(x) = x_i, \tag{23}$$

for every $i = 1, \dots, n-1$. Note that $f_n'(x) \leqq 1 - |\Sigma|/n + |\Sigma|/n = 1$, so that for $x \in (x_{i-1}, x_i)$ we have

$$f_n(x) - x_{i-1} = \int_{x_{i-1}}^{x} f_n'(t)\, dt \leqq x - x_{i-1},$$

and, therefore, $f_n(x) \leqq x$, which implies (23) and the injectivity of f_n. Finally, the sequence of simple deformations $n \mapsto (\kappa_n, f_n)$ satisfies

$$\liminf_{n \to +\infty} \kappa_n = \emptyset,$$

$$\lim_{n \to \infty} \| f_n - id \|_{L^\infty} \leqq \lim_{n \to \infty} \left(\frac{|\Sigma|}{n} \frac{1}{n} + \frac{1}{2} |\Sigma| \frac{1}{n^2} \right) = 0,$$

$$\lim_{n \to \infty} \| f_n' - 1 \|_{L^\infty} \leqq \lim_{n \to \infty} 2 \frac{|\Sigma|}{n} = 0,$$

and

$$\lim_{n \to \infty} \| f_n'' - \Sigma \|_{L^\infty} = 0.$$

Thus, $n \mapsto (\kappa_n, f_n)$ determines the second-order stuctured deformation $(\emptyset, \mathrm{id}, 1, \Sigma)$, where id denotes the identity function on $(0, 1)$.

We now specify a few items required for the statements and proofs of the Approximation Lemma and the Approximation Theorem for second-order structured deformations. These follow closely the specifications on pp. 130–131 of [1] for the case of first-order structured deformations. Let a piecewise-fit region $\mathcal{A}$ in $\mathbb{R}^N$ be given, and choose a Cartesian coordinate system for $\mathbb{R}^N$ satisfying $\overline{\mathcal{A}} \subset (1/3, 2/3)^N$. For each prime number p and each subset Z of the integers $\mathbb{Z}$, put

$$\Pi(p, Z) := \{\pi \ : \ \pi \text{ is a coordinate plane whose distance from the origin O is } m/p \text{ for some } m \in Z\}. \tag{24}$$

Let a second-order structured deformation of the form $(\emptyset, i, H, \Theta)$ be given, and choose sets $\{\mathcal{H}_j \ : \ j = 1, \dots, J\}$ as in (Std 2); in particular, the union of the sets $\mathcal{H}_j$ is the region $\mathcal{A}$, the restriction $H \mid_{\mathcal{H}_j}$ has a continuously differentiable extension to $\overline{\mathcal{H}_j}$, and the restriction $\Theta \mid_{\mathcal{H}_j}$ has a continuous extension to $\overline{\mathcal{H}_j}$, for $j = 1, \dots, J$. Choose a subdivision $\mathbf{B}$ of the piecewise fit region $\mathcal{A}$ into mutually disjoint fit regions $\mathcal{B}_j$, $j = 1, \dots, J$, whose union differs from $\mathcal{A}$ by a set of volume zero. (See the construction (3.17), [1], with $\mathcal{A}_j$ there replaced by $\mathcal{H}_j$.) Finally, we define

$$\Gamma(\mathbf{B}) := \bigcup_{j=1}^{J} \left((\partial \mathcal{B}_j) \cap \mathcal{A} \right)$$

and, for each $\varepsilon > 0$,

$$\Gamma(\mathbf{B})_\varepsilon := \{x \in \Gamma(\mathbf{B}) : \operatorname{dist}(x, \partial\mathcal{A}) < \varepsilon\}.$$

Lemma 1 (Approximation Lemma (cf. [1], p. 131)**).** *Let a piecewise fit region $\mathcal{A}$ and a second-order structured deformation $(\emptyset, i, H, \Theta)$ from $\mathcal{A}$ be given, choose sets $\{\mathcal{H}_j : j = 1, \ldots, J\}$ as in* (Std 2) *and a subdivision* **B** *as described above. For each $\varepsilon > 0$ and each prime number p, there exists a simple deformation (λ, h) from $\mathcal{A}$ and primes p_1, p_2 greater than p such that*

(i) *λ is covered by the set $\Gamma(\mathbf{B})_\varepsilon$ together with the planes $\pi \in \Pi(p_l, \{1, \ldots, p_l - 1\})$ with $l \in \{1, 2\}$;*
(ii) *$\|h - i\|_{L^\infty} < \varepsilon$;*
(iii) *$\|\nabla h - H\|_{L^\infty} < \varepsilon$;*
(iv) *$\|\nabla^2 h - \Theta\|_{L^\infty} < \varepsilon$.*

Moreover, (λ, h), p_1, and p_2 can be chosen so that, if

$$\mathcal{G} := \{x \in \mathcal{A} : H(x) = I, \Theta(x) = 0\}^\circ,$$

then $\lambda \cap \mathcal{G} = \emptyset$ and $h|_{\mathcal{G}} = i_{\mathcal{G}}$.

Proof. We note first that, by (Std 3), there exists $m > 0$ such that

$$m < \det H(x) \leqq \det \nabla i = 1 \tag{25}$$

for all $x \in \mathcal{A}$. Let $\varepsilon > 0$ and a prime p be given, and choose $\beta > 0$ such that

$$1 - \frac{\varepsilon}{4 \sup_{x \in \mathcal{A}} \|H(x)\|} < \beta < 1. \tag{26}$$

Let $H_j : \overline{\mathcal{H}_j} \to \mathbb{M}^{N\times N}$ and $\Theta_j : \overline{\mathcal{H}_j} \to \mathbb{M}^{N\times N\times N}$ denote the continuously differentiable and continuous extensions to the closure of $\mathcal{H}_j$ of H and Θ, respectively, described above. We note that $\max_{j=1,\ldots,J} \max_{x\in\overline{\mathcal{H}_j}} \|H_j(x)^{-1}\Theta_j(x)\| = 0$ if and only if $\Theta_j(x) = 0$ for every $x \in \mathcal{H}_j$ and for every $j = 1, \cdots, J$, and, without loss of generality, we may assume $\max_{j=1,\ldots,J} \max_{x\in\overline{\mathcal{H}_j}} \|H_j(x)^{-1}\Theta_j(x)\| > 0$ (otherwise, the proof of the present lemma reduces to that of the Approximation Lemma for first-order structured deformations). For each $j = 1, \ldots, J$ and $x \in \overline{\mathcal{H}_j}$, we define a quadratic mapping $f_j(x, \cdot) : \mathbb{R}^N \to \mathbb{R}^N$ by

$$f_j(x, y) := \tfrac{1}{2}\Theta_j(x)[y - x, y - x] + \beta H_j(x)(y - x) + x. \tag{27}$$

Putting $\Xi := \Theta_j(x)$, $A := \beta H_j(x)$, $a := x$, and $M := 1$, in view of (25) we may apply Theorem 1 to choose $r_j(x) > 0$ such that the restriction of $f_j(x, \cdot)$ to the ball $\mathcal{B}(x, r_j(x))$ has an extension to all of $\mathbb{R}^N$ as a C^2 diffeomorphism. Moreover the continuous dependence of $r_j(x)$ on $\Theta_j(x)$ and $H_j(x)$ established in Theorem 1, the uniform continuity of H_j and Θ_j, and the relations (25) and (26) tell us that:

(a)

$$\rho := \min_{j=1,\ldots,J} \min_{x\in\overline{\mathcal{H}_j}} r_j(x) > 0; \tag{28}$$

(b) we may choose a number δ for which

$$0 < \delta < \min\left\{\frac{\varepsilon}{4\sup_{x\in\mathcal{A}}\|\Theta(x)\|}, \frac{\varepsilon}{4\beta\sup_{x\in\mathcal{A}}\|H(x)\|}, \sqrt{\frac{\varepsilon}{2\sup_{x\in\mathcal{A}}\|\Theta(x)\|}}, 2\rho\right\} \tag{29}$$

and such that, if $x, y \in \overline{\mathcal{H}_j}$ and $\|x-y\| < \delta$, then

$$\|H_j(x) - H_j(y)\| \leqq \frac{\varepsilon}{2J}, \tag{30}$$

$$\|\Theta_j(x) - \Theta_j(y)\| \leqq \frac{\varepsilon}{2J}, \tag{31}$$

for every $j = 1, \ldots, J$.

For each such j we set

$$r_2^{(j)} := \inf_{x\in\overline{\mathcal{H}_j}} \inf_{y\in\partial\mathcal{B}(x,\delta/2)} \|f_j(x,y) - x\|, \tag{32}$$

and we now show that $r_2^{(j)} > 0$. By the compactness of $\overline{\mathcal{H}_j}$ we may choose sequences $n \mapsto x_n \in \overline{\mathcal{H}_j}$ and $n \mapsto y_n \in \partial\mathcal{B}(x_n, \delta/2)$ converging to $x_0 \in \overline{\mathcal{H}_j}$ and $y_0 \in \partial\mathcal{B}(x_0, \delta/2)$, respectively, such that $\|f_j(x_n, y_n) - x_n\|$ converges to $r_2^{(j)}$. Suppose $r_2^{(j)} = 0$. Then $f_j(x_n, y_n) - x_n \to 0$, so that $f_j(x_n, y_n) \to x_0$ as $n \to +\infty$. By (27), $f_j : \overline{\mathcal{H}_j} \times \mathbb{R}^N \to \mathbb{R}^N$ is continuous and we conclude that

$$f_j(x_0, x_0) = x_0 = \lim_{n\to+\infty} f_j(x_n, y_n) = f_j(x_0, y_0).$$

Because $f_j(x_0, \cdot)$ is injective on $\overline{\mathcal{B}(x_0, r_j(x_0))}$ and $x_0, y_0 \in \overline{\mathcal{B}(x_0, r_j(x_0))}$ we have $x_0 = y_0$, which contradicts the relation $y_0 \in \partial\mathcal{B}(x_0, \delta/2)$. Hence $r_2^{(j)} > 0$. We may now put

$$r_2 := \min_{j=1,\ldots,J} r_2^{(j)} > 0.$$

Choose a prime number p_1 such that

$$p_1 > \max\left\{p + 1, \frac{\sqrt{N}}{r_2}, \frac{2\sqrt{N}}{\delta}, \frac{2\sqrt{N}}{\varepsilon}\right\}, \tag{33}$$

and define $\mathbf{C}$ as the set of all closed cubes $\mathcal{C}$ in $(0,1)^N$ whose pairs of parallel faces are subsets of consecutive coordinate planes in $\Pi(p_1, \{1, \ldots, p_1 - 1\})$ as defined in (24). For each closed cube $\mathcal{C} \in \mathbf{C}$, we consider two cases:

(a) $\mathcal{C}$ is included in $\mathcal{A}$,
(b) $\mathcal{C}$ is neither included in nor disjoint from $\mathcal{A}$.

Case (a). Let $\mathcal{C} \in \mathbf{C}$ be given such that $\mathcal{C} \subset \mathcal{A}$. Using (30) and (31), it can be shown (cf. (5.35) of [1]) that if $x, y \in \mathcal{C}$, then

$$\|H(x) - H(y)\| \leqq \frac{\varepsilon}{2}, \tag{34}$$

$$\|\Theta(x) - \Theta(y)\| \leqq \frac{\varepsilon}{2}. \tag{35}$$

Choose $c_{\mathcal{C}}$ an arbitrary point in the cube $\mathcal{C}$, and define $f_{\mathcal{C}} : \mathbb{R}^N \to \mathbb{R}^N$ by

$$f_{\mathcal{C}}(x) := \tfrac{1}{2}\Theta(c_{\mathcal{C}})[x - c_{\mathcal{C}}, x - c_{\mathcal{C}}] + \beta H(c_{\mathcal{C}})[x - c_{\mathcal{C}}] + c_{\mathcal{C}}. \tag{36}$$

By the choice of the number ρ in (28), the mapping $f_{\mathcal{C}}$ restricted to the ball $\mathcal{B}(c_{\mathcal{C}}, \rho)$ is invertible. Since by (33) we have $\sqrt{N}/p_1 < \min\{\delta/2, r_2\}$, we may conclude that

$$\mathcal{C} \subset \mathcal{B}\left(c_{\mathcal{C}}, \frac{\delta}{2}\right) \cap f_{\mathcal{C}}\left(\mathcal{B}\left(c_{\mathcal{C}}, \frac{\delta}{2}\right)\right). \tag{37}$$

To show that $\mathcal{C} \subset f_{\mathcal{C}}\left(\mathcal{B}\left(c_{\mathcal{C}}, \frac{\delta}{2}\right)\right)$ we note that, otherwise, we may choose $x \in \mathcal{C}$ such that $x \neq f_{\mathcal{C}}(y)$ for all $y \in \mathcal{B}\left(c_{\mathcal{C}}, \frac{\delta}{2}\right)$. But $c_{\mathcal{C}} \in \mathcal{C} \cap \mathcal{B}\left(c_{\mathcal{C}}, \frac{\delta}{2}\right)$ and $c_{\mathcal{C}} = f_{\mathcal{C}}(c_{\mathcal{C}})$ so that the line segment through x and $c_{\mathcal{C}}$ is contained in $\mathcal{C}$, $c_{\mathcal{C}} \in f_{\mathcal{C}}\left(\mathcal{B}\left(c_{\mathcal{C}}, \frac{\delta}{2}\right)\right)$, but the end point x is not in $f_{\mathcal{C}}\left(\mathcal{B}\left(c_{\mathcal{C}}, \frac{\delta}{2}\right)\right)$. Because $f_{\mathcal{C}}$ is a diffeomorphism we may choose $\widetilde{x}$ on the line segment and $\widetilde{y} \in \partial\mathcal{B}\left(c_{\mathcal{C}}, \frac{\delta}{2}\right)$ such that $f_{\mathcal{C}}(\widetilde{y}) = \widetilde{x}$, and by (32), (33), and the definition of r_2,

$$r_2 > \|\widetilde{x} - c_{\mathcal{C}}\| = \|f_{\mathcal{C}}(\widetilde{y}) - c_{\mathcal{C}}\| \geqq r_2$$

a contradiction. From (29) we have that

$$f_{\mathcal{C}}\left(\mathcal{B}\left(c_{\mathcal{C}}, \frac{\delta}{2}\right)\right) \subset f_{\mathcal{C}}\left(\mathcal{B}\left(c_{\mathcal{C}}, \rho\right)\right). \tag{38}$$

Hence, $\mathcal{C}$ is a subset of the range of $f_{\mathcal{C}}$ which is equal to the domain of $f_{\mathcal{C}}^{-1}$, and, by (37), we also have that

$$f_{\mathcal{C}}^{-1}(\mathcal{C}) \subset \mathcal{B}\left(c_{\mathcal{C}}, \frac{\delta}{2}\right). \tag{39}$$

Recall that $\det H(x) \leqq 1$ for every $x \in \mathcal{A}$, so that $\det(\beta H(c_{\mathcal{C}})) < 1$. Thus, by (20), we have $0 < \det \nabla f_{\mathcal{C}}(x) < 1$ for every $x \in \mathcal{B}(c_{\mathcal{C}}, \rho)$ and, therefore, $\det \nabla f_{\mathcal{C}}^{-1}(x) > 1$ for every $x \in f_{\mathcal{C}}(\mathcal{B}(c_{\mathcal{C}}, \rho))$, so that $\mathrm{vol}(\mathcal{C}) < \mathrm{vol}(f_{\mathcal{C}}^{-1}(\mathcal{C}))$. Proceeding as in pp. 133–134 of [1], it can be shown that there exists a prime $p_{\mathcal{C}}$ such that for every prime $p' > p_{\mathcal{C}}$ there exists an injective, piecewise rigid mapping $r_{\mathcal{C}} : \mathcal{C}\backslash\Pi(p', \mathbb{Z}) \to f_{\mathcal{C}}^{-1}(\mathcal{C}^\circ)$. We define the set

$$\lambda_{\mathcal{C}} := \{x \in \pi \cap \mathcal{C}^\circ : \pi \in \Pi(p', \{1, \ldots, p' - 1\})\}$$

and the mapping $h_{\mathcal{C}} : \mathcal{C}^\circ\backslash\lambda_{\mathcal{C}} \to \mathcal{C}^\circ$ by

$$h_{\mathcal{C}}(x) := f_{\mathcal{C}}(r_{\mathcal{C}}(x)).$$

We now check that on its domain the map $h_{\mathcal{C}}$ satisfies the requirements (ii), (iii), (iv). We first note by (39) that $r_{\mathcal{C}}(x) \in \mathcal{B}\left(c_{\mathcal{C}}, \frac{\delta}{2}\right)$ for every $x \in \mathcal{C} \subset \mathcal{B}\left(c_{\mathcal{C}}, \frac{\delta}{2}\right)$, so that

$$\|r_{\mathcal{C}}(x) - x\| \leqq \delta \tag{40}$$

for every $x \in \mathcal{C}$. By using (36), (40), (29), and (33)–(35) we see that

$$\begin{aligned}
\|h_{\mathcal{C}}(x) - i(x)\| =\; & \|\tfrac{1}{2}\Theta(c_{\mathcal{C}})[r_{\mathcal{C}}(x) - c_{\mathcal{C}}, r_{\mathcal{C}}(x) - c_{\mathcal{C}}] \\
& + \beta H(c_{\mathcal{C}})[r_{\mathcal{C}}(x) - c_{\mathcal{C}}] + c_{\mathcal{C}} - x\| \\
\leqq\; & \tfrac{1}{2}\|\Theta(c_{\mathcal{C}})\|\delta^2 + \beta\|H(c_{\mathcal{C}})\|\delta + \frac{\sqrt{n}}{p_1} \leqq \frac{\varepsilon}{4} + \frac{\varepsilon}{4} + \frac{\varepsilon}{2} = \varepsilon, \\
\|\nabla h_{\mathcal{C}}(x) - H(x)\| =\; & \|\Theta(c_{\mathcal{C}})[r_{\mathcal{C}}(x) - c_{\mathcal{C}}] + \beta H(c_{\mathcal{C}}) - H(x)\| \\
\leqq\; & \|\Theta(c_{\mathcal{C}})\|\delta + (1-\beta)\|H(c_{\mathcal{C}})\| + \|H(c_{\mathcal{C}}) - H(x)\| \leqq \varepsilon,
\end{aligned}$$

and

$$\|\nabla^2 h_{\mathcal{C}}(x) - \Theta(x)\| = \|\Theta(c_{\mathcal{C}}) - \Theta(x)\| \leqq \varepsilon.$$

Case (b). This case can be analyzed by following the argument above and the argument on pp. 134–135 of [1], and we only outline the reasoning here. Let a cube $\mathcal{C} \in \mathbf{C}$ be given such that $\mathcal{C} \cap \mathcal{A} \neq \emptyset$ and $\mathcal{C} \cap (\mathbb{R}^N \backslash \mathcal{A}) \neq \emptyset$. Let $\mathbf{B} = \{\mathcal{B}_1, \ldots, \mathcal{B}_J\}$ be the subdivision of $\mathcal{A}$ chosen just above the statement of this lemma, and for every $j = 1, \ldots, J$ we put

$$\mathcal{C}_j = \overline{\mathcal{B}}_j \cap \mathcal{C}, \tag{41}$$

we choose $y_j \in \mathcal{C}_j$, and define $f_{\mathcal{C}_j} : \mathbb{R}^N \to \mathbb{R}^N$ by

$$f_{\mathcal{C}_j}(x) = \tfrac{1}{2}\Theta(y_j)[x - y_j, x - y_j] + \beta H(y_j)[x - y_j] + y_j.$$

Using the same procedure as described above we can choose a prime $p_{\mathcal{C}_j}$ such that, for all primes $p_j' \geqq p_{\mathcal{C}_j}$, there exists an injective piecewise rigid mapping $r_{\mathcal{C}_j}$ which maps $\mathcal{C}_j \backslash \Pi(p_j', \mathbb{Z})$ into $f_{\mathcal{C}_j}^{-1}\left(\mathcal{C}_j^\circ\right)$. We now define

$$\begin{aligned}
\lambda_{\mathcal{C}_j} &= \{x \in \pi \cap \mathcal{C}_j^\circ \,:\, \pi \in \Pi(p_j', \{1, \ldots, p_j' - 1\})\}, \\
h_{\mathcal{C}_j}(x) &= f_{\mathcal{C}_j}(r_{\mathcal{C}_j}(x)),
\end{aligned}$$

for $x \in \mathcal{C}_j \backslash \lambda_{\mathcal{C}_j}$.

Using the pairs $(\lambda_{\mathcal{C}_j}, h_{\mathcal{C}_j})$ we can construct a simple deformation from $\mathcal{C}^\circ \cap \mathcal{A}$ that satisfies (ii)–(iv), and the construction of the simple deformation (λ, h) satisfying (i)–(iv) in the statement of the lemma can be done, using the simple deformations constructed above and following the reasoning on p. 136 of [1]; verification of the "Moreover..." assertion at the end of this lemma follows the argument on pp. 136 and 137. □

The factorization of the type (16),

$$(\kappa, g, G, \Sigma) = (\emptyset, i, H, \Theta) \circ (\kappa.g), \tag{42}$$

where

$$H(y) = (G(\nabla g)^{-1})(g^{-1}(y)) \tag{43}$$

and

$$\begin{aligned}\Theta(y)[a, b] = {} & \Sigma(g^{-1}(y))[(\nabla g)^{-1}(g^{-1}(y))a, (\nabla g)^{-1}(g^{-1}(y))b] \\ & - (G(\nabla g)^{-1})(g^{-1}(y))\nabla^2 g(g^{-1}(y))[a, b]\end{aligned} \tag{44}$$

for every $y \in g(\mathcal{A}\backslash\kappa)$ and $a, b \in \mathbb{R}^N$, together with Proposition 1, permits us to deduce from the Approximation Lemma the existence of a determining sequence for each second-order structured deformation. The details of the argument follow those on pp. 138–139 of [1] and provide the desired proof of our main result:

Theorem 2 (Approximation Theorem for Second-Order Structured Deformations**).** *For each piecewise fit region $\mathcal{A}$ and second-order structured deformation (κ, g, G, Σ) from $\mathcal{A}$, there exists a sequence $m \mapsto (\kappa_m, f_m)$ of simple deformations from $\mathcal{A}$ that determines (κ, g, G, Σ).*

It is convenient to use the term "disarrangement" [4] to denote non-classical geometrical changes due to slip and separation on internal surfaces and occurring possibly at more than one length scale. Because ∇f_m and $\nabla^2 f_m$ do not measure such geometrical changes, it is natural in view of the Approximation Theorem to call $G = \lim_{m\to\infty} \nabla f_m$ the (*first-order*) *deformation without disarrangements* and $\Sigma = \lim_{m\to\infty} \nabla^2 f_m$ the (*second-order*) *deformation without disarrangements* for the second-order structured deformation (κ, g, G, Σ). Because κ_m is a collection of points where f_m can fail to be smooth, we call κ_m the *disarrangement site* for the simple deformation (κ_m, f_m) and, in view of the Approximation Theorem, we call $\kappa = \liminf_{m\to\infty} \kappa_m$ the (*permanent*) *disarrangement site* for the second-order structured deformation (κ, g, G, Σ). Measures of deformation due to disarrangement for second-order structured deformations will be identified in the next section.

4. Decompositions and identification relations

We recall from relation (5) that the Approximation Theorem for first-order structured deformations and a Gauss-Green formula imply the "identification relation":

$$\begin{aligned} M(x) &:= \nabla g(x) - G(x) \\ &= \lim_{r\to 0} \lim_{m\to+\infty} \frac{1}{\mathrm{vol}(B(x, r))} \int_{B(x,r)\cap\Gamma(f_m)} [f_m](y) \otimes \nu_{\Gamma(f_m)}(y)\, d\mathcal{A}_y, \end{aligned} \tag{45}$$

where $\Gamma(f_m)$ denotes the jump-set for f_m, $[f_m](y)$ denotes the jump in f_m at $y \in \Gamma(f_m)$, $\nu_{\Gamma(f_m)}(y)$, denotes the normal at the point $y \in \Gamma(f_m)$, and $\mathcal{A}_y$ denotes N-dimensional area measure. The term "identification relation" is appropriate for the formula (45), because it identifies the difference $M(x) = \nabla g(x) -$

$G(x) = (\nabla \lim_{m\to\infty} f_m - \lim_{m\to\infty} \nabla f_m)|_x$ as a measure of deformation due to a large number of small jumps in f_m. This identification relation justifies calling $\nabla g(x) - G(x)$ the (*first-order*) *deformation due to* (*micro*) *disarrangements* [5]. For a second-order structured deformation (κ, g, G, Σ) we have, by the Approximation Theorem, $\nabla G = \nabla \lim_{m\to\infty} \nabla f_m$ and $\Sigma = \lim_{m\to\infty} \nabla^2 f_m = \lim_{m\to\infty} \nabla(\nabla f_m)$; the results in [2] when applied to ∇f_m, instead of to f_m, then yield a new identification relation:

$$\begin{aligned}&\nabla G(x) - \Sigma(x) \\ &= \lim_{r\to 0} \lim_{m\to+\infty} \frac{1}{\mathrm{vol}\,(B(x,r))} \int_{B(x,r)\cap\Gamma(\nabla f_m)} [\nabla f_m](y) \otimes \nu_{\Gamma(\nabla f_m)}(y)\, d\mathcal{A}_y.\end{aligned} \tag{46}$$

Here, for each $A \in \mathrm{Lin}(\mathbb{R}^N)$ and $v \in \mathbb{R}^N$, we define the tensor product $A \otimes v \in \mathrm{Lin}(\mathbb{R}^N, \mathrm{Lin}(\mathbb{R}^N))$ by $(A \otimes v)w = Aw \otimes v$ for all $w \in \mathbb{R}^N$. The identification relation (46) permits us to call $\nabla G(x) - \Sigma(x)$ a (*second-order*) *deformation due to disarrangements*. If we differentiate both sides of the identification relation (45) and add the resulting equation to the identification relation (46), we obtain the identification relation

$$\begin{aligned}&\nabla^2 g(x) - \Sigma(x) = \nabla G(x) - \Sigma(x) + \nabla M(x) \\ &= \lim_{r\to 0} \lim_{m\to+\infty} \frac{1}{\mathrm{vol}(B(x,r))} \int_{B(x,r)\cap\Gamma(\nabla f_m)} [\nabla f_m](y) \otimes \nu_{\Gamma(\nabla f_m)}(y)\, d\mathcal{A}_y \\ &\quad + \nabla_x \lim_{r\to 0} \lim_{m\to+\infty} \frac{1}{\mathrm{vol}(B(x,r))} \int_{B(x,r)\cap\Gamma(f_m)} [f_m](y) \otimes \nu_{\Gamma(f_m)}(y)\, d\mathcal{A}_y.\end{aligned} \tag{47}$$

In this relation, we may call $\nabla^2 g(x) - \Sigma(x)$ a (second-order) deformation due to disarrangments, and this difference is revealed as the term $\nabla G(x) - \Sigma(x)$ arising only from jumps in ∇f_m plus the term $\nabla M(x)$ arising only from jumps in f_m. We may now write

$$\begin{aligned}\nabla g(x) &= G(x) + M(x), \\ \nabla^2 g(x) &= \nabla G(x) - \Sigma(x) + \nabla M(x) + \Sigma(x),\end{aligned}$$

and use relation (8) to obtain the *refined quadratic approximation:*

$$\begin{aligned}g(x) - g(y) = {} & G(x)(y-x) + M(x)(y-x) \\ & + \tfrac{1}{2}(\nabla G(x) - \Sigma(x))[y-x, y-x] + \tfrac{1}{2}\nabla M(x)[y-x, y-x] \\ & + \tfrac{1}{2}\Sigma(x)[y-x, y-x] + o(|y-x|^2).\end{aligned} \tag{48}$$

In this approximation, the terms $G(x)(y-x)$ and $\frac{1}{2}\Sigma(x)[y-x, y-x]$ represent *translations without disarrangements*, from limits of first gradients ∇f_m and second gradients $\nabla^2 f_m$, respectively. The terms $M(x)(y-x)$, $\frac{1}{2}(\nabla G(x) - \Sigma(x))[y-x, y-x]$, and $\frac{1}{2}\nabla M(x)[y-x, y-x]$ represent *translations due to disarrangements*: $M(x)(y-x)$ and $\frac{1}{2}\nabla M(x)[y-x, y-x]$ arise due to jumps in f_m, whereas $\frac{1}{2}(\nabla G(x) - \Sigma(x))[y-x, y-x]$ arises due to jumps in ∇f_m.

5. Additional examples

Example 2 (Bending through simple shears). Let $N = 2$ and let $\mathcal{A} = (0, 1) \times (0, 1)$. For each positive integer n, put $y_i := i/n$ for $i = 0, 1, \ldots, n$, and $\kappa_n := \{(0, 1) \times \{y_i\} : i = 1, 2, \ldots, n-1\}$. Let $h \in C^2((0, 1); \mathbb{R})$, and for $i = 0, 1, \ldots, n-1$ define

$$m_i := \frac{h(y_{i+1}) - h(y_i)}{y_{i+1} - y_i},$$

as well as

$$h_n(y) := \sum_{i=0}^{n-1} (m_i(y - y_i) + h(y_i))\, \chi_{(y_i, y_{i+1})}(y).$$

Finally, we put $f_n(x, y) := (x + h_n(y), y)$ and $g(x, y) := (x + h(y), y)$. It is easily seen that the simple deformation (κ_n, f_n) determines the second-order structured deformation $(\emptyset, g, \nabla g, 0)$. Moreover, M vanishes, and the translations due to disarrangements in (48) arise solely from the term $\nabla G - \Sigma = \nabla^2 g$, whose only non-zero component is $\nabla^2 g(x, y)_{122} = h''(y)$. In view of (46), the translations due to disarrangements associated with $(\emptyset, g, \nabla g, 0)$ arise through the jumps in ∇f_n, specifically, the jumps in h_n'.

Example 3 (Bending of a deck of cards). Let $N = 2$ and let $\mathcal{A} = (-1, 1) \times (2, 3)$. For each positive integer n, put $y_i := 2 + \frac{i}{n}$ for $i = 0, 1, \ldots, n$, and $\kappa_n := \{(-1, 1) \times \{y_i\} : i = 1, 2, \ldots, n-1\}$. We define

$$\rho(y) := \sqrt{1 + y^2} \tag{49}$$

and

$$f_n(x, y) := \frac{\rho(y)}{\rho([ny]/n)}(x, \sqrt{\rho([ny]/n)^2 - x^2}) \tag{50}$$

for every $(x, y) \in (-1, 1) \times (2, 3)$. Here, $[\cdot]$ denotes the greatest integer function, and relation (50) tells us that lines $y = y_0$ are mapped by f_n into circular arcs with center at the origin and radius $\rho(y_0)$, while lines $x = x_0$ are mapped into a collection of line segments, each of which, when extended, passes through the origin. Figure 1 shows the effect of the mapping f_n on rectangles of the form $(-1, 1) \times (y_i, y_{i+1})$: each is mapped into an annular region with inner radius $\rho(y_i)$ and outer radius $\rho(y_{i+1})$. (This deformation is reminiscent of the geometrical changes in a deck of cards when it is bent prior to shuffling.) Because $0 \leqq y - [ny]/n \leqq 1/n$, it follows that $\rho([ny]/n)$ converges to $\rho(y)$ as n tends to infinity, uniformly in y. Consequently, the sequence $n \mapsto f_n$ converges uniformly on $(-1, 1) \times (2, 3)$ to the function g defined by

$$g(x, y) := (x, \sqrt{1 + y^2 - x^2}), \tag{51}$$

and the gradients

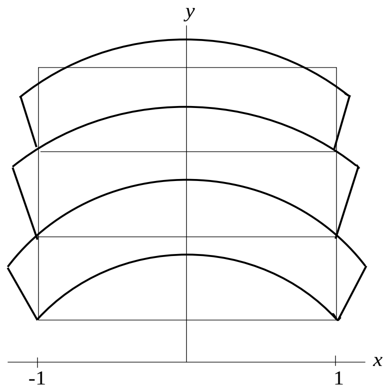

Fig. 1. Microview of the deformation of Example 3.

$$\nabla f_n(x, y) = \begin{bmatrix} \frac{\rho(y)}{\rho([ny]/n)} & \frac{xy}{\rho([ny]/n)\rho(y)} \\ -\frac{\rho(y)x}{\rho([ny]/n)\sqrt{\rho([ny]/n)^2-x^2}} & \frac{y}{\rho([ny]/n)\rho(y)}\sqrt{\rho([ny]/n)^2 - x^2} \end{bmatrix}$$

converge uniformly to

$$G(x, y) := \begin{bmatrix} 1 & \frac{xy}{1+y^2} \\ -\frac{x}{\sqrt{1+y^2-x^2}} & \frac{y\sqrt{1+y^2-x^2}}{1+y^2} \end{bmatrix}. \tag{52}$$

We easily find that

$$\nabla g(x, y) = \begin{bmatrix} 1 & 0 \\ -\frac{x}{\sqrt{1+y^2-x^2}} & \frac{y}{\sqrt{1+y^2-x^2}} \end{bmatrix} \tag{53}$$

and, therefore, on $(-1, 1) \times (2, 3)$, we have

$$\frac{2}{3} \leqq \frac{y}{\sqrt{1 + y^2 - x^2}} = \det G(x, y) = \det \nabla g(x, y).$$

Consequently, the inequalities in (Std 3) of Definition 3 are satisfied by G and ∇g. Finally, the second gradients $\nabla^2 f_n$ are easily shown to converge uniformly to the tensor field Σ having components Σ_{ijk} at (x, y) given by

$$\Sigma_{111} = 0, \qquad \Sigma_{112} = \frac{y}{1 + y^2},$$

$$\Sigma_{121} = \frac{y}{1 + y^2}, \qquad \Sigma_{122} = \frac{x}{(1 + y^2)^2},$$

$$\Sigma_{211} = -\frac{1 + y^2}{(1 + y^2 - x^2)^{3/2}}, \qquad \Sigma_{212} = -\frac{xy}{\sqrt{1 + y^2 - x^2}(1 + y^2)},$$

$$\Sigma_{221} = -\frac{xy}{\sqrt{1 + y^2 - x^2}(1 + y^2)}, \qquad \Sigma_{222} = \frac{\sqrt{1 + y^2 - x^2}}{(1 + y^2)^2},$$

and it is straightforward to verify that $\nabla G \neq \Sigma$, $\nabla M \neq 0$, and $\nabla^2 g \neq \Sigma$. Thus, the second-order structured deformation deformation $(\emptyset, g, G, \Sigma)$ represents a macroscopic bending of the two-dimensional region $(-1, 1) \times (2, 3)$, with accompanying disarrangements occurring due to jumps both in f_n and in ∇f_n.

Acknowledgements. We wish to acknowledge the support of the Center for Nonlinear Analysis, Department of Mathematical Sciences, Carnegie Mellon University, as well as the support of the National Science Foundation under Grant DMS 9703863 awarded to David R. Owen. We also thank Irene Fonseca for valuable comments that improved the exposition of our results, and Stephane Pagano for help in preparing Fig. 1.

References

1. G. Del Piero, & D. R. Owen, Structured deformations of continua, *Arch. Rational Mech. Anal.* **124**, 99–155 (1993).
2. G. Del Piero & D. R. Owen, Integral-gradient formulae for structured deformations, *Arch. Rational Mech. Anal.* **131**, 121–138 (1995).
3. W. Noll & E. Virga, Fit regions and functions of bounded variation, *Arch. Rational Mech. Anal.* **102**, 1–22 (1988).
4. D. R. Owen, Disarrangements in continua and the geometry of microstructure, in *Recent Advances in Elasticity, Viscoelasticity, and Inelasticity*, pp. 67–81, ed., K. Rajagopal, World Scientific, Singapore, 1995.
5. G. Del Piero & D. R. Owen, *Structured Deformations*, Lecture Notes, XXII Scuola Estiva di Fisica Matematica, Ravello, September, 1997. Research Report No. 99-CNA-014, Center for Nonlinear Analysis, Department of Mathematical Sciences, Carnegie Mellon.
6. R. Choksi & I. Fonseca, Bulk and interfacial energy densities for structured deformations of continua, *Arch. Rational Mech. Anal.* **138**, 37–103 (1997).
7. R. Choksi, G. Del Piero, I. Fonseca, & D. Owen, Structured deformations as energy minimizers in models of fracture and hysteresis, *Mathematics and Mechanics of Solids,* **4**, 321–356 (1999).
8. I. Fonseca, G. Leoni, & R. Paroni, A note on Meyers' theorem in $W^{k,1}$, in preparation.
9. I. Fonseca, G. Leoni, & R. Paroni, Relaxation in $BH(\Omega; R^d)$, in preparation.
10. I. Fonseca, G. Leoni, & R. Paroni, in preparation.

Department of Mathematical Sciences
Carnegie Mellon University
Pittsburgh, PA 15213-3890

and

Dipartimento di Ingegneria Civile
Università degli Studi di Udine
Via della Scienze 208
33100 Udine, Italy

(*Accepted Juni 1, 2000*)
Published online November 24, 2000 –