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Original Article

From Finite Element Stress Maps to Defensible Aligner Prescriptions: A Methodological Framework for Model Credibility, Biological Applicability, and Uncertainty in Periodontally Compromised Dentitions

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ABSTRACT

Clear-aligner finite element analysis can resolve stresses, strains, displacements, and force-system responses that are difficult to measure directly, but numerical detail does not by itself justify a clinical prescription. This distinction becomes especially important in periodontally compromised dentitions, where altered attachment support changes mechanical behavior while biological tolerance remains incompletely represented by most computational models. This methodological framework examines the inferential steps required to move from simulated clear-aligner outputs toward clinically defensible interpretation. It distinguishes model construction from model credibility, identifies major sources of uncertainty arising from anatomy, material behavior, appliance fit, attachment design, boundary conditions, treatment staging, and periodontal support, and separates verification of computational implementation from validation against physical or clinical observations. The framework further treats biological applicability as an additional requirement rather than an automatic consequence of mechanical agreement. The central proposition is that simulation claims should be graded according to what the model has actually demonstrated: prediction of a modeled mechanical state, correspondence with measurable mechanical behavior, or applicability to a defined clinical context. In periodontally compromised dentitions, a stress map can therefore inform biomechanical reasoning without automatically establishing a safe displacement, optimal activation, or treatment protocol. Greater clinical influence requires stronger evidence connecting modeled assumptions, validation targets, patient-specific support conditions, and residual uncertainty. This approach preserves the analytical value of finite element modeling while limiting unjustified translation from numerical outputs to patient-level prescriptions.

Keywords: Clear aligners, Finite element analysis, Periodontal support, Model credibility, Biomechanical validation, Uncertainty

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Introduction

Clear-aligner biomechanics are produced by interacting properties of the appliance, dentition, programmed movement, material behavior, attachment configuration, and supporting tissues. Contemporary reviews therefore describe clear-aligner mechanics as strongly conditional rather than as a uniform force-delivery system [1]. Finite element analysis (FEA) has become one of the principal methods used to examine these interactions because it can estimate local displacements, stresses, strains, and force-system responses that are difficult to isolate experimentally. Yet a recent systematic review of clear-aligner FEA identified substantial methodological heterogeneity across published models, including differences in geometric representation, material assumptions,

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contact definitions, loading strategies, and reported outcomes [2]. The existence of increasingly detailed simulations has consequently not eliminated the problem of deciding what those simulations are entitled to mean clinically.

The distinction between a numerically resolved output and a credible clinical inference is well established in the broader field of biomedical modeling. Credible modeling practice requires an explicit context of use, appropriate verification and validation activities, assessment of uncertainty, transparent documentation, and limits on claims that exceed the evidence supporting the model [3]. Validation is likewise not an all-or-none property of a model. It is tied to the intended application, the observable used for comparison, the conditions under which the model is tested, and the consequence of relying on the resulting prediction [4]. A model that satisfactorily reproduces one measurable mechanical response may remain unvalidated for another output, another patient configuration, or a biological outcome occurring over a different timescale.

These distinctions are especially consequential in periodontally compromised dentitions. Reduced alveolar support changes the geometry through which orthodontic loads are transmitted, while clinical decision-making must account simultaneously for inflammation control, attachment loss, tissue response, tooth movement objectives, appliance behavior, and longitudinal monitoring. A computational stress concentration or displacement pattern may therefore be biomechanically informative without identifying a clinically acceptable activation. Similarly, a lower predicted stress does not automatically establish biological safety, and a configuration that appears mechanically favorable cannot be interpreted as superior treatment without evidence extending beyond the modeled system.

This article develops a methodological framework for determining when clear-aligner FEA can support increasingly consequential clinical claims. The analysis first defines the methodological foundations of aligner FEA, then identifies major sources of model uncertainty, before distinguishing verification, validation, and biological applicability and integrating those distinctions into a claim-specific model-credibility framework. The aim is not to reject computational biomechanics, nor to construct a numerical treatment threshold, but to clarify the evidentiary steps that must separate a simulated stress map from a defensible aligner prescription.

Methodological foundations of aligner finite element modeling

A finite element model is a structured representation of a physical system rather than a digital duplicate of the patient. Its usefulness depends on whether the aspects retained in the representation are sufficient for the question being asked. In clear-aligner modeling, this normally requires geometric representations of teeth and supporting structures, an aligner or equivalent appliance geometry, defined contact or bonding relationships, constitutive descriptions for modeled materials, boundary conditions, and a specified activation or displacement. The resulting solution describes the behavior of that constructed system under those assumptions. It does not independently establish that the same forces, strains, or tissue responses occur in vivo.

Experimental validation work illustrates both the value and the limits of such models. Ye and colleagues compared finite element predictions with micro-computed tomographic measurements of aligner-tooth gaps and digital image correlation measurements of aligner surface strains, demonstrating close correspondence for selected mechanical observables within the tested configuration [5]. This type of comparison is methodologically important because it tests whether a modeled mechanical behavior can reproduce an independently measured physical behavior. It does not, however, transform strain agreement into validation of periodontal remodeling, long-term tooth movement, patient comfort, or treatment success. The validation domain remains the domain that was actually measured.

Hybrid computational and experimental designs can strengthen this connection. Jin and colleagues evaluated posterior reinforcement during anterior retraction using both finite element analysis and an experimental model with force and moment measurements [6]. Such work provides a more defensible basis for interpreting the simulated force system than simulation alone because at least part of the modeled behavior is confronted with physical measurement. Even so, bench correspondence remains a mechanical validation step. It cannot substitute for biological or clinical validation when the eventual claim concerns treatment response in living tissues.

The temporal representation of treatment introduces another methodological layer. Conventional FEA often represents an immediate mechanical state: an activation is imposed and the resulting response is calculated. Clear-aligner therapy, however, involves sequential appliances, changing geometry, incomplete tracking, viscoelastic behavior, and repeated loading.

Mao and colleagues used an iterative four-dimensional finite element approach to simulate staged maxillary premolar distalization, demonstrating that predicted movement changes as sequential treatment states are incorporated [7]. Iterative methods can therefore address some limitations of a single static calculation, but computational staging should not be equated with biological time. Recalculation after a simulated movement does not, by itself, reproduce periodontal ligament adaptation, bone remodeling, inflammation, individual wear behavior, or variable appliance seating.

Appliance design further illustrates why model inputs are inseparable from model outputs. In a finite element investigation of maxillary incisor torque, different auxiliary configurations produced different displacement and stress patterns even though the therapeutic objective was similar [8]. Likewise, alternative programmed movement strategies for correcting a deep curve of Spee produced materially different anterior biomechanical responses [9]. These findings do not identify universally preferable configurations. They demonstrate a more fundamental methodological point: a stress or displacement map is conditional on the modeled intervention architecture. Changing the auxiliary, activation, movement sequence, or contact relationship changes the mechanical problem being solved.

The same principle applies to simplification. Every finite element model omits details. The relevant question is not whether simplification exists, but whether the omitted properties can materially affect the output used to support a particular claim. A model designed to compare relative aligner deformation may require a different level of periodontal representation from one intended to estimate tissue-level loading in a severely reduced periodontium. Similarly, a representation sufficient for exploratory comparison between two attachment shapes may be inadequate for a prescription-level conclusion about a specific patient's allowable activation. Model adequacy must therefore be judged against the intended inference rather than against a single universal standard of geometric or computational complexity.

This relationship between model purpose, assumptions, and interpretability is summarized in **Table 1**. The table treats each assumption as a methodological choice whose acceptability depends on the output being interpreted, rather than automatically classifying simplification as error.

Table 1. Model assumptions that condition the interpretation of clear-aligner finite element outputs

Model component	Typical modeling decision	Why the assumption matters biomechanically	Interpretation that may remain defensible	Claim that requires stronger evidence
Tooth and root geometry	Patient-specific or idealized anatomy	Alters contact geometry, lever arms, displacement pattern, and local support relationships	Comparison within the modeled geometry	General patient-level prescription
Periodontal ligament	Simplified constitutive behavior and thickness	Influences load transfer and calculated stress/strain fields	Relative mechanical comparison under stated assumptions	Prediction of biological tolerance or remodeling
Alveolar support	Full or reduced support geometry	Changes effective support, mobility tendency, and stress concentration	Support-specific mechanical interpretation	Universal activation threshold for periodontal patients
Aligner material	Selected elastic or viscoelastic representation	Influences stiffness, deformation, and force transmission	Behavior of the specified material model	Exact in-mouth force history without validation
Aligner–tooth contact	Idealized contact, friction, or fitted interface	Determines seating, engagement, slipping, and load transmission	Conditional comparison between modeled interfaces	Assumption that programmed movement equals delivered loading
Attachments and auxiliaries	Geometry, placement, or omission	Changes moment generation, retention, and movement control	Configuration-specific force-system analysis	Clinical superiority of a design
Programmed activation	Prescribed displacement or staged movement	Defines the imposed mechanical challenge	Response to that modeled activation	Safe or optimal clinical increment
Boundary and anchorage conditions	Fixed, constrained, or auxiliary-supported structures	Redistributes displacement and reaction forces	Scenario-specific biomechanical comparison	Direct transfer to another anchorage configuration

Treatment time representation	Static or iterative/staged analysis	Determines whether changing geometry is represented	Mechanical response across simulated states	Complete representation of biological treatment time

Sources of model uncertainty

Model uncertainty in clear-aligner FEA is not a single residual error that can be appended to a result after calculation. It originates at multiple stages: geometry acquisition, constitutive modeling, appliance representation, contact definition, activation, boundary conditions, numerical implementation, and the translation from mechanical output to biological interpretation. These uncertainties may interact. A highly refined mesh does not compensate for an inappropriate material law, and patient-specific tooth geometry does not resolve uncertainty about periodontal tissue behavior or aligner seating.

Material representation is a prominent example. Clear-aligner polymers differ in composition, stiffness, processing, thickness, thermoforming behavior, water sensitivity, viscoelasticity, and time-dependent relaxation. Reviews of contemporary aligner materials demonstrate that these properties can change during fabrication and use and that a nominal material description cannot be assumed to represent a constant in-mouth mechanical state [10]. A model that assigns one elastic modulus to an aligner may be appropriate for a narrow comparative purpose, but uncertainty rises when the same output is interpreted as a direct estimate of force maintained over days of clinical wear.

Geometry at the appliance margin also affects transmission. A systematic review of aligner trimline and extension designs found that variations in gingival extension and trimline configuration influence biomechanical behavior, although the underlying studies remain heterogeneous [11]. This creates uncertainty not only about which geometric representation is selected but also about whether the digital model adequately represents actual seating, trimming, deformation, and gingival interaction. A computationally precise aligner with an idealized interface may therefore give a highly reproducible answer to a physical problem that differs from the appliance worn by the patient.

Patient and tooth morphology create another layer of uncertainty. Finite element analyses indicate that clinical crown length can alter predicted incisor displacement and periodontal ligament stress [12]. Attachment location and design similarly change rotational mechanics, stress distribution, and aligner deformation in modeled premolars [13]. These findings make patient geometry scientifically relevant, but they do not imply that increasing geometric personalization removes uncertainty. A patient-specific surface mesh may still be paired with assumed tissue properties, simplified contacts, uncertain appliance fit, or incompletely characterized periodontal support.

The distinction becomes particularly clear when simulation is compared with clinical observation. In a real-case based study of maxillary molar distalization, Chen and colleagues compared finite element predictions under different anchorage designs with observed tooth movement and found broad agreement for several movements but a notable discrepancy in the behavior of the central incisors [14]. The important methodological lesson is not that the model “worked” or “failed.” Rather, validation can be local. Agreement for one tooth, displacement direction, or mechanical output does not authorize the assumption that every modeled output is equally credible.

Initial treatment configuration also changes the mechanical question. Different starting posterior inclinations during extraction-space closure generated different displacement patterns and centers of rotation in finite element analysis [15]. Palatal anchorage configuration likewise altered predicted molar distalization and periodontal ligament stresses [16]. These studies show why boundary conditions must be treated as part of the scientific hypothesis rather than as incidental model settings. A result obtained under one anchorage or inclination condition cannot be transferred to another simply because the same aligner technology is used.

Scenario dependence becomes even more pronounced when several treatment features interact. Torque overcorrection during mandibular incisor intrusion produces different predicted responses under extraction and non-extraction conditions [17]. In extraction models, changing anterior spacing alters the predicted balance between incisor intrusion, tipping, and periodontal ligament loading [18]. Attachment designs also change modeled control during molar mesialization [19]. Collectively, these findings argue against interpreting isolated numerical outputs as intrinsic characteristics of a movement such as intrusion, retraction, rotation, or mesialization. The output belongs to a defined configuration of anatomy, appliance design, activation, anchorage, and assumptions.

A useful uncertainty analysis should therefore ask which uncertainties can be reduced, which can be quantified or explored through sensitivity analysis, and

which remain structural limitations of the model. Mesh convergence can address numerical discretization uncertainty, but it cannot establish that tissue constitutive assumptions are biologically correct. Experimental comparison may validate an aligner deformation or force component while leaving periodontal response untested. Patient-specific geometry can improve anatomical fidelity while retaining uncertainty regarding tissue properties. Clinical comparison can strengthen credibility for selected outcomes but may expose disagreement elsewhere. These distinctions are summarized in **Table 2** and will form the basis for separating verification from validation and biological applicability in the next section.

Table 2. Uncertainty sources and the corresponding credibility questions in clear-aligner finite element modeling

Uncertainty source	Where it enters the model	Mechanically affected interpretation	Appropriate credibility question	What would remain unresolved after a favorable check
Image-derived anatomy	Segmentation and geometric reconstruction	Root position, crown geometry, support relationships	Is the represented anatomy sufficiently accurate for the intended output?	Tissue behavior and treatment response
Periodontal support geometry	Bone-height and support representation	Center of resistance, displacement tendency, local loading	Does the modeled support condition represent the clinical state being discussed?	Biological tolerance to the resulting loading
Mesh and numerical discretization	Element type, size, convergence	Numerical stability and local stress estimates	Is the solution sufficiently insensitive to further discretization?	Model-form and biological uncertainty
Aligner material law	Elastic/viscoelastic constitutive assumptions	Force magnitude, deformation, relaxation	Does the constitutive representation reproduce relevant material behavior?	Individual in-mouth aging and wear history
Appliance fit and contact	Interface, friction, seating, trimline	Engagement and force transmission	Does the contact formulation reproduce relevant physical behavior?	Patient-specific tracking throughout treatment
Attachments and auxiliaries	Geometry, location, constraints	Moments, retention, rotational and translational control	Are mechanical effects reproduced for the tested configuration?	Comparative clinical effectiveness
Programmed activation	Prescribed displacement or movement sequence	Entire calculated force system	Is the imposed activation representative of the actual mechanical challenge?	Whether the patient receives or tolerates that activation biologically
Anchorage and boundary conditions	Fixed or constrained structures	Reaction forces and displacement distribution	Are the constraints defensible for the clinical scenario?	Transferability to another anchorage arrangement
Initial tooth configuration	Inclination, spacing, extraction state	Centers of rotation and movement coupling	How sensitive is the output to clinically plausible starting states?	Generalization beyond those states
Simulated treatment progression	Static versus iterative updates	Time/state dependence of predicted mechanics	Does staged updating improve mechanical representation?	True periodontal remodeling and long-horizon biological adaptation
Clinical comparison	Observed versus simulated displacement	External correspondence of selected outputs	Does the specified outcome agree under the tested patient and treatment conditions?	Validity of unmeasured outputs, other patients, or biological safety

The uncertainty structure developed here does not imply that every clear-aligner model must reproduce every biological detail. It instead establishes a proportionality principle: the closer a simulation is brought to a patient-level prescription, the more consequential its unresolved assumptions become. A model may be entirely useful for comparing two attachment configurations while remaining insufficient

for declaring one configuration safer for a periodontally compromised patient. The next analytical step is therefore not to demand unrealistic completeness, but to determine which aspects of the computational system have been verified, which modeled responses have been validated, and whether those validated responses are biologically applicable to the clinical claim being made.

Verification, validation, and biological applicability

Verification, validation, and biological applicability answer different questions and should not be collapsed into a single claim that a finite element model is "validated." Verification concerns whether the computational implementation solves the intended mathematical and numerical problem with sufficient consistency. Validation asks whether specified outputs correspond to independent observations under defined conditions. Biological applicability asks whether those validated outputs can legitimately inform the tissue state, patient population, treatment stage, and clinical decision under consideration. Progress through these levels is therefore conditional rather than automatic.

This distinction becomes critical as periodontal support is reduced. Ma and Li demonstrated that changing periodontal support within a finite element model alters predicted periodontal ligament stresses and tooth displacement [20]. Their study supports the mechanical premise that loss of support changes the modeled response. It does not establish a universal biologically safe displacement increment. A numerical displacement associated with a favorable stress pattern in one modeled dentition remains conditional on its geometry, constitutive assumptions, loading representation, and the absence of direct prospective validation against periodontal outcomes.

Clinical evidence imposes another boundary. An international Delphi study examining indications and limitations of clear-aligner therapy identified areas of agreement while retaining uncertainty for clinically complex situations, including compromised periodontal conditions [21]. A separate international consensus investigation similarly recognized substantial therapeutic potential alongside biomechanical and clinical limitations [22]. Consensus can inform cautious practice where evidence is incomplete, but agreement among experts is not equivalent to verification of a computational model or validation of a predicted periodontal response.

The problem also extends beyond periodontal severity itself. Finite element studies of anterior torque during extraction treatment show that the resulting displacement and stress fields depend on the particular torque strategy modeled [23]. En-masse retraction simulations demonstrate that Class II elastics and anchorage mechanics redistribute movement and reaction forces [24]. Comparisons of strong anchorage strategies in bimaxillary extraction models likewise produce different biomechanical responses across treatment configurations [25]. These studies are useful because they identify mechanical contingencies; they become unsafe only when a configuration-specific prediction is presented as if it were a transportable prescription.

Clinically interpretable simulation therefore requires a chain of evidence rather than a favorable stress map. **Table 3** defines the minimum evidentiary questions that should be answered before progressively stronger claims are made.

Table 3. Evidentiary requirements for increasingly consequential interpretations of clear-aligner finite element simulations

Intended claim	Minimum evidence required before interpretation	Residual uncertainty that must remain explicit	Claim language that remains defensible
The computational solution behaves consistently	Numerical verification, mesh or solution stability, transparent boundary and contact definitions	Model-form and biological uncertainty	"The model predicts…"
One modeled design differs mechanically from another	Verified computation with comparable assumptions and controlled model changes	Dependence on selected geometry, material laws, and activation	"Under the modeled conditions…"
A simulated output represents measurable appliance behavior	Comparison with independent mechanical measurements relevant to that output	Untested outputs and patient variability	"The predicted mechanical response corresponded with…"
A predicted tooth movement corresponds with observed movement	Output-specific comparison with clinical or experimental displacement data	Other teeth, movements, patients, treatment stages, and biological response	"Agreement was observed for…"

A model is applicable to reduced periodontal support	Explicit representation of support loss plus evidence that the relevant mechanical outputs remain credible in that state	Tissue remodeling, inflammatory status, individual susceptibility, longitudinal response	"The model supports biomechanical interpretation in the represented support condition…"
A simulation informs a clinical prescription	Verified model, relevant validation, biologically appropriate population, credible treatment context, quantified or transparently discussed uncertainty	Residual patient-specific and biological uncertainty	"The simulation may inform, but does not independently determine, clinical prescription…"

The resulting boundaries are summarized in **Figure 1**. The important transition is not from a "low" to a "high" stress value, but from one category of inference to another.

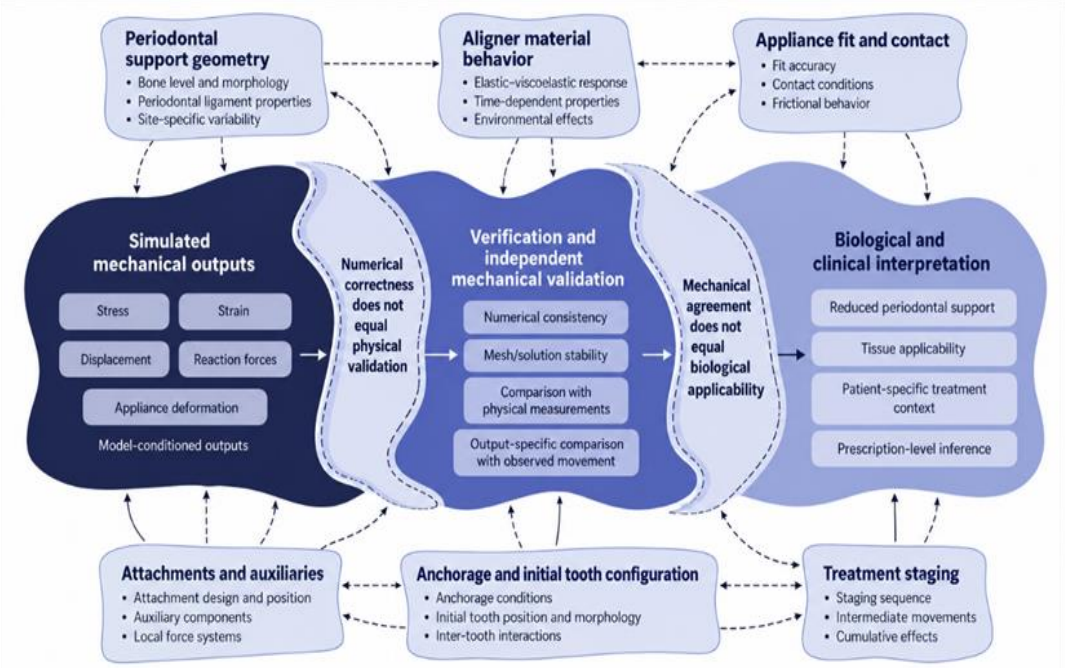


Figure 1. Credibility boundaries across simulated mechanics, validation, and periodontal interpretation

A model-credibility framework for clinical translation

The evidentiary burden placed on a model should depend on what the model is being asked to influence. In medical-device simulation, credibility frameworks explicitly connect model risk to the consequence of relying on the computational result [26]. The same logic can be adapted cautiously to clear-aligner biomechanics. A simulation used to explore whether changing an attachment alters a local force system does not require the same credibility evidence as a simulation used to justify a patient-specific activation in a periodontally reduced dentition.

Recent work on credibility assessment for in-silico clinical trials further emphasizes that computational credibility must be tied to a defined context of use and evaluated through a structured sequence rather than inferred from model sophistication alone [27]. In clear-aligner FEA, context of use should state the intended clinical or scientific question, the population and periodontal condition represented, the output being interpreted, the decision that the output may influence, and the consequence of error.

On this basis, the present framework treats translation as an evidence chain. First, the model must be sufficiently well specified to make the simulated quantity interpretable. Second, numerical behavior must be verified. Third, the relevant mechanical output should be validated wherever an independent comparator is available. Fourth, the biological and periodontal conditions represented in the model must be compatible with the clinical claim. Finally, residual uncertainty must remain visible when the result is communicated. A break at one level restricts the strength of the downstream claim rather than invalidating every use of the model.

Figure 2 represents this adjudication process. It is deliberately nonlinear because deficiencies in material representation, fit, support geometry, validation evidence, or biological applicability can each force a

claim to be narrowed even when other parts of the model are strong.

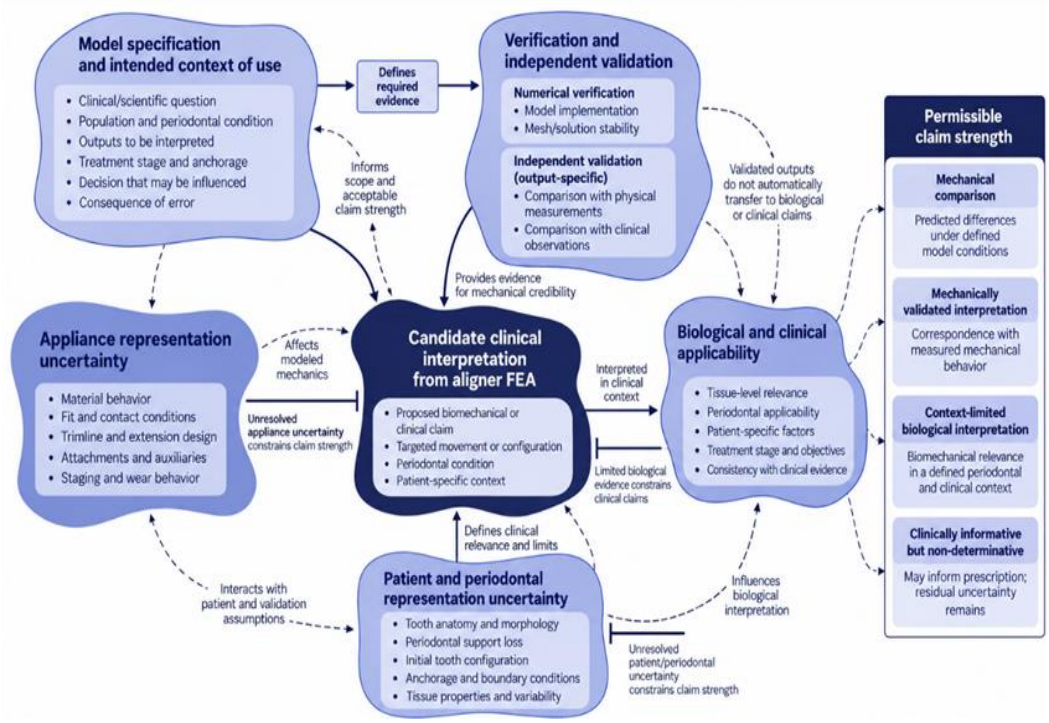


Figure 2. Uncertainty adjudication before a clear-aligner simulation can support a clinical claim

Reporting standards, clinical implications, and limitations

Clear-aligner FEA should be reported at the level required for readers to reconstruct the intended inference, not merely the numerical procedure. At minimum, reports supporting clinically relevant claims should describe anatomy and periodontal support representation, aligner and attachment geometry, material assumptions, contact conditions, activation strategy, anchorage, boundary conditions, mesh and numerical checks, validation targets, and important sensitivity analyses. Uncertainty that is known but not quantified should still be identified explicitly.

Claim wording should also reflect evidentiary status. Stress, strain, and displacement maps may justify statements about predicted mechanical behavior under defined model conditions. Agreement with independent mechanical measurements can justify stronger statements about those particular outputs. Neither level alone demonstrates biological safety, periodontal stability, superior clinical effectiveness, or an optimal activation. Terms such as *safe*, *optimal*, *effective*, or *recommended* should therefore be reserved for circumstances in which evidence extends beyond relative simulation rankings.

For periodontally compromised dentitions, this restraint is clinically productive rather than merely conservative. Reduced support changes the mechanical environment, but periodontal treatment status, inflammatory control, tissue morphology, patient adherence, and longitudinal remodeling are not reducible to a stress contour. FEA can help identify scenarios deserving caution, expose sensitivity to support loss, compare alternative mechanical configurations, and formulate testable hypotheses. It is less defensible as an autonomous prescriber.

The framework has limitations. Much of the aligner literature available for model comparison remains simulation based, and validation frequently concerns only selected mechanical observables. Patient-specific models may improve anatomical representation without eliminating uncertainty in tissue constitutive behavior, appliance seating, wear, or biological adaptation. Furthermore, general credibility frameworks developed for physiological modeling and medical-device simulation require orthodontic adaptation rather than direct transplantation. These limitations support a graded approach to credibility: models should be judged according to their intended clinical influence and the evidence available for that use.

Conclusion

Finite element analysis is valuable because it makes otherwise inaccessible aspects of clear-aligner

mechanics examinable, but numerical resolution does not itself confer clinical authority. In periodontally compromised dentitions, defensible interpretation requires explicit separation of computational verification, output-specific validation, and biological applicability. Material behavior, geometry, appliance fit, attachments, anchorage, staging, and periodontal support can each alter the model's answer, while clinical relevance depends on whether those modeled conditions correspond to the patient and decision under consideration. The most defensible use of aligner FEA is therefore claim-specific: simulation can compare mechanical scenarios, generate hypotheses, and support biomechanical reasoning, while prescription-level conclusions require stronger evidence and transparent residual uncertainty. A credible model should narrow uncertainty without concealing the boundary between what has been simulated, what has been validated, and what remains a clinical inference.

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