



WORLDWIDE NEWS

May 2004

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Articles

4	RIM --Ami Ben-Bassat's Blog - A New Israeli test confirms: PEI (Pidgeon Enabled Internet) is FASTER then ADSL
7	MSC.Software: Success Story Simulation Reduces Airline Seat Testing Costs at B/E Aerospace
10	AVI and Website: www.fluid-structureinteraction.com Fluid Flow Between Two Glasses - Alexey I. Borovkov, Igor B. Voinov
11	ETA: eta/VPG Software
13	FEA Participant listing
14	May participants websites to visit
15	Events & Previous News Page
16	Invitation from Ismail Mehmet Yeyinmen, Ph.D. Chairman of BYM Group
Publication	8th International LS-DYNA Users Conference May 2-4, 2004 Investigation of dsDNA Stretching Meso-Mechanics Using LS-DYNA

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RIM --Ami Ben-Bassat's Blog
A New Israeli test confirms:
PEI (Pidgeon Enabled Internet) is FASTER then ADSL

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Pigeons beat ADSL



Will B2B (Back to Pigeons) save an endangered technology? On Friday, March 12, 2004, a group of several dozen Internet addicts from Israel and abroad, gathered in the large grass field of the OHALO Center near the Sea of Galilee. The purpose of the gathering was to try and improve **Wi-Fly** - pigeon-empowered wireless internet and to confront this technology against ADSL. The participants sent 3 homing pigeons to 100 km distance, each carrying 20-22 tiny memory cards containing 1.3 GB, amounting in total of 4 GB of data.

Dr. Yossi Vardi, with Ami Ben-Bassat, a science writer, and Guy Vardi, the CPO (chief pigeon/technical officer) conceived and run the test. The purpose of the test was to measure and confirm an improvement over the pi[ge]oneering method, conceived by David Waitzman and first implemented several years ago in Bergen, Norway.

"Improving the method was achieved by changing the medium on which the message is stored and carried by the pigeons, from paper (as required by the original protocol) to Memory Flash Cards", said Ben Bassat. Replacing the old analog content transfer by **digital** one, enables the **pigeons to transfer data faster than ADSL**, and to achieve what apparently looks as pigeons' record in data transfer to a given distance.

"Never underestimate a pigeon carrying a memory card, hovering above your head, ready to download"-yossi vardi

TCP (Transmission by Carrier Pigeons) properties:

Operating System

After careful analysis it was found that although Linux is better liked by penguins, nevertheless, Windows may totally crash the avian system and may be fatal. In case your pigeons are flying on Windows it may be wise to use precautions. According one manufacturer, using screen-saver may avoid Windows-kill. It also should be noted that pigeons had other usages in the internet (see Google's own pigeonRank technology), as well as other birds, such as ducks (racing ducks), penguins, etc.



flipping the bird to ADSL

Infrastructure

No external sources of energy, such as batteries or electrical extension cords are needed! The technology eliminates the need for cat 5 or fiber-optic cables (cat 5 or any cat among the pigeons is not recommended any how). No relay stations are needed for the Wi-Fly transmission.

Security

As was proven already in World War II, even when using PGP (Pretty Good Pigeons), pigeons are susceptible to hacking. The technology is susceptible to Denial of Service. According some manufacturers, homing pigeons works well with certain firewalls

Privacy

Pigeons are less likely than a regular ISP to cooperate, willingly or unwillingly, with the RIAA in surrendering the names of young customers who are involved with file sharing, therefore they provide higher level of privacy for P2P (*Disclaimer: The owners of this site are in no way advocating, any illegal, immoral or fattening activities. All information provided here is for research, educational, scientific, humaniterian and pigeonierian purposes only*).

Marketing

The technology opens new opportunities for branding and marketing.

Latency

Latency is much higher: no matter how little data will be transferred, it will take longer for the first bit to arrive. Nevertheless, for a distance of few hundreds km pigeons' latency is shorter than that of Netflix, Fedex, or the postal service.

Scalability

Infrastructure Scalability is achieved by natural replication. Increasing data rate transfer capacity, rather than being subject, as in similar cases to Gilder's law, is subject to Moor's law. Resolving Feynman's challenge will increase it further.

Routing and routers

Pigeons are using their own proprietary ultra-efficient flying micro-routers which have not been deciphered so far. However, routing may be subject to interference from cellular towers, and with other birds.



flying data

Setting records: apparently three records have been accomplished during the test:

I Pigeons' Data Transfer Rate:

Calculating the bandwidth by dividing the amount of data by the flying time of the last pigeon, show that the bandwidth achieved by the pigeons was significantly larger than that available through commercially available ADSL broadband Internet connections: about 2.27 Mbps (Mega bit per second) as compared to 0.75 – 1.5 Mbps. [*Please note that all measured times are of an observer on the ground. If measured by the moving pigeon it self, times are a bit shorter, according to Einstein's relativity theory*].

II Elegant solution- Maximum data transfer throughput per mass of infrastructure:

The developers of the new method followed Buckminster Fuller's Ephemeralization notion – doing more with less. Numerous proposals have been made in the past to ship data by brute force e.g., by station wagon, camels, Boeing 747 etc, but the developers are not aware of any technological means to transfer the said amount of data to a given destination with less mass of infrastructure, and energy (3 Pigeon-Power). Hence, as far as the developers of the new method are aware, the suggested method set a record also to that respect.



Scalability achieved by natural replication

III Pigeons' Wi-Fly has longer range than Wi-Fi:

The wireless Wi-Fly range which was demonstrated, was much higher than of Wi-Fi, even if the Wi-Fi is enhanced with the improved Pringles-Potato-Chips-Canister Antenna.

Defense Applications

Concluding the event, Dr. Yossi Vardi, summed up by saying that in addition to the three above mentioned records, Pigeons-Empowered Internet has number of merits over conventional internet: The technology doesn't suffer from electricity interruptions. It is naturally rechargeable by the carrier itself, using commonly available materials. If a pigeon fails to perform in the internet-it always can be put to secondary usage.

However, the technology, admittedly, suffers from few disadvantages: First, they may be radioactive hazards. Second, since pigeons do not fly at night, this method's bandwidth drops to zero at those times. The third and foremost is that unlike pigeons, ADSL doesn't shit on your head, or on your car.

[Fallback: In a case of emergency when you can't find pigeons, you may try to use chickens or pigs. As a solution of last resort you may retreat to Bongo Drums]

MSC.Software Success Story Simulation Reduces Airline Seat Testing Costs at B/E Aerospace
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All airline seats must be certified to meet FAA airworthiness standards with physical test data. Currently, the FAA requires certification data to be derived from destructive physical tests, which are time consuming and expensive. When a test failure occurs and multiple tests are required, the cost of additional physical testing is substantial and can jeopardize the aircraft delivery schedule.

B/E Aerospace Inc., the leading manufacturer of commercial aircraft seating, has successfully used MSC.Patran and MSC.Nastran simulation tools when a seat has not met the certification test criteria to determine the causes and suggest design revisions. This has reduced the number of subsequent physical tests to just one, saving upwards of one week and \$35,000 per test.

The FAA certification tests require a fully occupied seat to withstand specified dynamic inertial loads. In addition, whole structures must withstand applied static loads. Dynamic loads are tested by mounting the seat and anthropomorphic test dummies on a sled. The sled simulates a crash by reaching a specified velocity and peak deceleration over a required period of time. The seat must withstand the loads, and the test dummy must meet the requirements for occupant safety.



Nastran Stress Plot of Seat Bracket

Roy Turvaville, Certification & Structures Engineer, said, "When the head strikes the seat in front, there are certain deceleration limits for that event, called the Head Injury Criterion (HIC), and we run a vertical test, where we measure loads on the spinal column of the test dummy. In addition, we are required to induce floor deformation onto the seat, so the seat is not just on a flat surface like on an aircraft. We rotate one leg 10 degrees then pitch the other leg 10 degrees in the opposite direction. Even before the test starts, a great deal of deformation and internal stresses take place in the seat structure. The minimum

accelerations for the structural test are 16G's, which is pretty severe, and it typically occurs in less than a 1/4 of a second."

Typically, MSC.Patran and MSC.Nastran virtual product development (VPD) tools are used for forensics when there is a test failure. The broken component is investigated to determine the contributing factors. MSC.Patran readily accepts the solid model geometry created in Unigraphics, which is B/E Aerospace's native CAD system, allowing a mesh to be created very quickly. The loads, proper boundary constraints, and material properties are applied in MSC.Patran. The analysis is then performed with MSC.Nastran. Simulation provides a much better understanding of how seats and components work during dynamic events. While a physical test is basically a pass/fail event, simulation provides engineers with data revealing how close to failure or how over-engineered a component is. Based on the analysis information, the part is redesigned, generally changing geometry by adding thickness or changing material. Then the entire seat must be tested again.

Mr. Turvaville said, "When there is a test failure, there is a lot of pressure to pass the next test because tests are time consuming and expensive. Each certification test destroys a production seat, so you don't want to run unnecessary tests. You don't want to run tests blindly, where you don't know what's really going on. Using the simulation software, we have a much better idea of how the seat structure is working during the dynamic events. And when we do have a failed test, very often we can have a design change and verify it on the same day."

Conducting a physical test event requires a seat and very complicated setup process. The seats must be inspected and documented, then mounted to the sled. The test dummy has to be mounted and in the proper position. Mr. Turvaville said, "If you have to change a part, you have to go to a machine shop and get a part made and put it on the seat. Depending on the part, it can be just a couple of days if it can be made locally. There can be three or four days involved, plus a lot of overhead and consumables and manpower in running the test which can add up to thousands of dollars for each test procedure. When you include the cost of a seat itself, and you destroy the seat during the test, the total cost escalates rapidly."



Typically, B/E Aerospace customers' aircraft are built in the United States, Germany, or France. The aircraft are built to a specific schedule, which requires the seats to be delivered at a specific time. If the test program is delayed because of test failures, there is a lot of pressure to pass the next test.

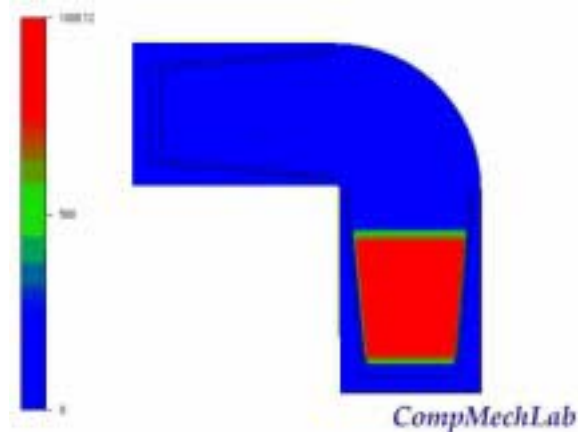
Mr. Turvaville said, "Since using simulation, we have a 100% pass rate on second tests. Without simulation, we could have three or four more tests to get a design that would work. Simulation has saved a lot of unnecessary tests and repetition of tests. Because of our successes with simulation, we've found it much easier to meet the delivery schedules, which have added to increased customer satisfaction."

Mr. Turvaville added, "Recently, FAA Draft Advisory Circular 25.562-1B has proposed allowing the use of computer simulation in place of physical testing. This would mean with a product, such as MSC.Dytran, we could further reduce the time and cost of airline seat certification."

Showcased Website and AVI
Website: www.fluid-structureinteraction.com
Alexey I. Borovkov, Igor B. Voinov
Flow of the fluid between two glasses

AVI Library 90 and 90a

CompMechLab



The problems of dynamic interaction of media in different aggregative states like rigid body and fluid/air are among the most interesting and sophisticated problems of mechanics.

The presented AVI files illustrate the behavior of the fluid during the flow between the glasses. The problem was solved with use of LS-DYNA code.

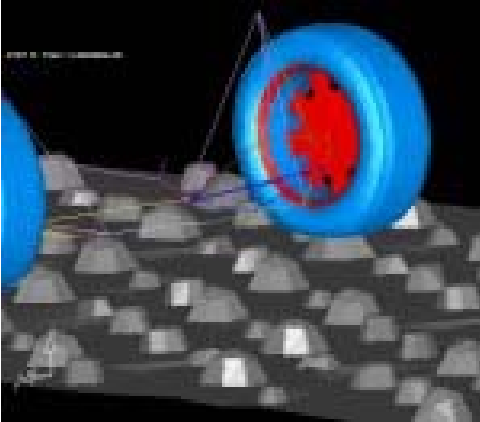
To simulate this and similar processes two element types with different formulation were used. The glasses were simulated as rigid bodies (MAT_RIGID). At this the equations of the motion are applied in the Lagrange formulation. The fluid and surrounding air are simulated by means of finite elements based on Euler formulation.

To describe the physical properties of the fluid the Newton equations of the viscous flow were applied together with the Gruneisen equation of state.

Contact interaction between the fluid and rigid body (glass) is simulated with use of special algorithm of the mutual penetration restriction for the two media described by different formulations of the motion equations (Lagrange and Euler). LS-DYNA card `CONSTRAINED_LAGRANGE_IN_SOLID` is used for this restriction.

In the first AVI file distribution of the densities in the considered space is presented. Red color corresponds to the spaces occupied by the fluid; blue color corresponds to air and green – to the boundary layer between fluid and air. In the second AVI file the fluid flow process is shown; free surface of the fluid is presented as equiscalar surface created based on density distribution.

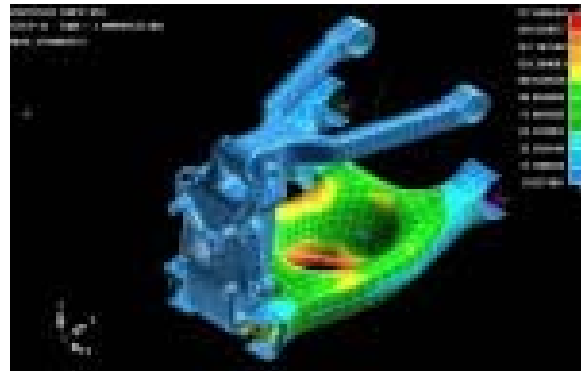
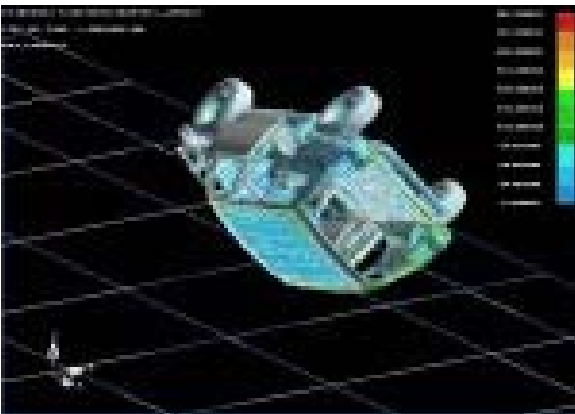
eta/VPG
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Integrated at an earlier stage of the design process, eta/VPG reduces time, reduces cost, and improves quality.

eta/VPG's unique analysis approach, allows the automotive industry to achieve its quest of reducing time-to-market and prototype costs

This streamlined CAE software package provides an event-based simulation solution of nonlinear, dynamic problems. eta/VPG's single software package overcomes the limitations of existing CAE analysis methods. It is designed to analyze the behavior of mechanical and structural systems as simple as linkages, and as complex as full vehicles.





DOWNLOAD VPG:

www.eta.com/Products/VPG/vpgdownload.html

VPG/PrePost has the most complete suite of meshing tools for all major finite element programs.

100% LS-DYNA , NASTRAN and RADIOSS interfaces allowing complete access to all features

Provides CAD data interfaces as well as state-of-the-art automeshing tools.

Advanced post processing tools directly access the results files for animations and x-y curve plotting

VPG/Structure allows users to create multi-body style models of mechanical systems.

Suspension templates allow users to create typical suspension models easily

Tire Models can be generated and integrated into your system model

Complexity can range from simple mechanism models to fully flexible structural system models of vehicles

VPG/Safety has 17 different FMVSS and ECE vehicle safety regulations coded into the software.

The unique "process guidance approach" used to set up models improves productivity and makes complicated simulations easier.

Contains a Crash Tool Library of barriers, dummies and impactor models which are used in simulations

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Participant Websites to Visit

<http://www.intel.com>

The screenshot shows the Intel website homepage. At the top left is the Intel logo. To its right are links for "US Home | Intel Worldwide" and "Where to Buy | Training". Below the logo is a navigation bar with five categories: "Resource Centers", "Products & Services", "Solutions", "Technologies & Trends", and "Support & Downloads". The "Resource Centers" section is expanded, listing: "Personal Computing" (Products and tools to help you buy or build the perfect PC), "Business/Enterprise" (Find products, solutions and strategies for the enterprise), "Hardware Design" (Tools and resources for hardware design and development needs), "Software Development" (Get technical resources: tools, code, training, forums, & support), and "Intel® Reseller Center" (Information designed to support the growth of Intel resellers). To the right of this list is a large blue banner with three circular images of people using laptops. The banner text reads: "Where Will You Unwire? Check e-mail from a public hotspot. Download MP3s or play online games in the living room. With Intel® Centrino™ mobile technology and a wireless connection, the possibilities are endless+." A "Learn More" button is at the bottom right of the banner.

<http://www.arup.com/dyna/>

The screenshot shows the Arup LS-DYNA Environment website. At the top left are links for "Global Home | Skills & Services | Offices | Careers". To the right is a search box with a "go" button. The Arup logo is in the top right corner. Below the logo is a blue banner with the text "Oasys LS-DYNA Environment". Underneath the banner is a navigation menu with links: "home", "applications", "software", "models", "downloads", "courses", "links", and "contact". Below the menu is a row of three images: a building, a yellow hard hat, and a wireframe model of a structure. At the bottom left, it says "Welcome to the Oasys LS-DYNA site,". At the bottom right, there is a blue button labeled "Latest News".

Special Announcements and Highlights of News Page

April 05	ANSYS – Multi Field Solver
	Flotrend – Distributor in Taiwan
April 12	Added AVI's to Warhead Analysis
	Special posting for LSTC on LS-DYNA Conference
April 19	The Japan Research Institute – LS-DYNA and related products
	SGI - SGI Altix 3000 servers and superclusters
	Dynamax – Distributor in US

EVENTS

2004	
May 24-26	2004 ANSYS Users Conference and Exhibition to be held in Pittsburgh, Pennsylvania, U.S.A.
Sept. 7-9	The Seventh International Conference on Computational Structures Technology, Lisbon, Portugal
Sept. 21-22	2004 Japanese LS-DYNA Users Conference hosted by JRI, will be held at Akasaka Prince Hotel in Tokyo.
Sept 26-28	ANSYS CHINA - Annual User Conference
Oct. 11-12	The Nordic LS-DYNA Users' Conference 2004 will be held at Quality Hotel 11, Goteborg
Oct.14-15	3rd local LS-DYNA Conference - Bamberg, Germany sponsored by DYNAMore
Oct. 18 - 20	MSC.Software's 2004 Americas Virtual Product Development Conference - October 18 - October 20 2004 Hyatt Regency Huntington Beach, CA, USA
Nov 10-12	22. CAD-FEM Users' Meeting 2004 - International Congress on FEM Technology & ANSYS CFX @ ICEM CFD Conference
2005	
May 25-26	5th European LS-DYNA Conference - The ICC, Birmingham UK
2006	
June	9th International LS-DYNA Users Conference – Dearborn, Michigan

OPEN INVITATION
From Ismail Mehmet Yeyinmen, Ph.D.
Chairman of BYM Group

BYM was established in 1989 to provide advanced technology "Solutions" in management and engineering. Today, BYM Group is rendering advanced technology services to automotive industry.

The mission of the group is to lead and move the Turkish automotive industry into a global platform of product and tool design as well as manufacturing. Also, to create and render technology training programs to lessen the shortages of qualified personnel in product and tool design.

In this context, 16 node 32 cpu Linux cluster has been built and LS-DYNA MPP version is operational as "Online Simulation Center" which is accessible free of charge by academia and students. Special training programs of LS-DYNA are offered along with adjunct graduate level courses with Department of Engineering, Marmara University, Istanbul. "Tooling Designer Certificate Program" is a 256 hour training course that has been implemented in collaboration with Engineering Department, Sakarya University, Sakarya with a scope of design fundamentals and basic implementation of know how for those engineers who desire to make a career in tool design.

With this message, we are inviting all Turkish engineers and designers using LS-DYNA to become honorary members of the "Online Simulation Center" of BYM Group contributing to the creation of the Global Simulation Network of Turkey. By the end of June 2004, a portal for this purpose will also be operational.

We will be pleased and grateful for your comments, suggestions and advice and thank you for your time and consideration in advance.

Respectfully
Ismail Mehmet Yeyinmen, Ph.D.
Chairman of BYM Group
imy@bym.net

Investigation of dsDNA Stretching Meso-Mechanics Using LS-DYNA

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Abstract

This paper proposes a novel mathematical model for studying the entropic elasticity and cooperative extensibility of double strand DNA (dsDNA) using LS-DYNA and equivalent theory. Through the proposed model, the dynamic structural transitions of the dsDNA under external force/torque can be accurately simulated within an affordable CPU time. Moreover, the proposed dsDNA model comprises the meso-mechanics equivalent theory of single molecule dsDNA, including the base-stacking interaction between DNA adjacent base pairs, the Hydrogen bond of complementary base-pairs and electrostatic interactions along double-helix sugar-phosphate backbones. Good agreement is achieved between the numerical simulation and the single molecular manipulation experimental result, and the mechanical behavior of stretching nicked dsDNA could be revealed.

Introduction

During the past decade, the single molecular manipulation technique has been developed to measure the basic physical properties of double stranded double-strand deoxyribose nucleic acid (dsDNA) and to discover the interaction between dsDNA and proteins/enzymes [1]. The structure of B-DNA has been first discovered by the Watson and Crick at 1950s. The blue two double helix chains indicate the sugar-phosphate backbone of DNA. The black rods represent the base pairs. Additionally, the red and green circles represent the hydrogen bonds between bases [1]. Moreover, the results of the nicked dsDNA stretching experiment have indicated that a sharp structural transition occurs under roughly 65pN of tension, and that the classical B-DNA structure dramatically transits to a S-DNA structure [3-5]. In Figure 2, (a) is the schematic illustration of the optical tweezers system, which can be used as a single-molecular manipulation. One end of dsDNA is fixed to the glass substrate; the other end is attached to the micro bead. (b) is the schematic illustration of B-DNA and S-DNA. S-DNA is proposed to be the ladder type structure. (c) is the single-molecular measurement result of stretching dsDNA, and abrupt structural transition (B-S transition) and the plateau of nicked dsDNA of 65 pN. (the experimental results are based on the [3])

However, the resolution of the single molecular measurement technique currently available restricts the researchers to completely clarify the mechanical behavior of stretching dsDNA as well as the continuous geometrical deformation of the sugar-phosphate chain during stretching. To conquer the resolution limitation of the single molecular dsDNA manipulation technique, the molecular biology researcher essentially requires accurate theoretical model to address the dsDNA mechanical characteristics under specific external loading and boundary condition. However, a feasible numerical model to describe the dsDNA mechanics is difficult to achieve, because the meso-mechanics of single-molecule dsDNA include both quantum mechanics and continuum mechanics. Benham [6] have derived the analytical wormlike rod chain model (WLRC model), and Marko et al. [7] have improved the accuracy of Benham's WLRC model.

These WLRC models could predict the DNA mechanical response under low level stretching. However, the WLRC model could not accurately describe the P-form and S-form DNA under high level stretching force or twisting torque. Zhou et al. [8] have proposed the unique Zhou, Zhang and Ou-Yang model (ZZO model), which considers the bending energy and the base pairs staking energy of dsDNA. The ZZO model could successfully describe the S-type DNA under high level stretching, but it could hardly represent the structural transition from the B-form DNA to the P-form DNA due to its limitation of geometric assumption. Additionally, these theoretical models mentioned above could not provide the dynamic dsDNA structural transition in virtuality. Therefore, the dynamic/transient finite element method with material/geometrical nonlinear properties is applied in this study in order to comprehensively understand the mechanical behavior of dsDNA under external loading.

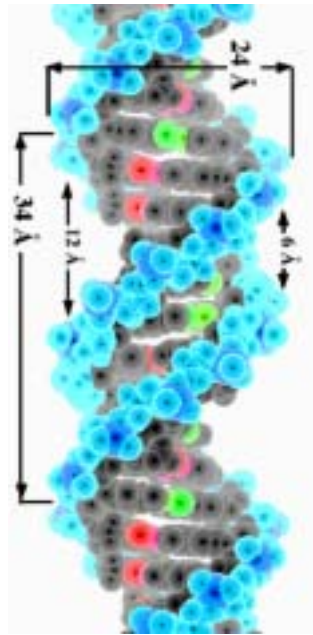


Figure 1. Schematic illustration of classic B-type dsDNA.

The finite element method considers the minimization of the total potential energy, which includes internal energy, bending energy, twisting energy, the contact energy and the external energy of dsDNA. Moreover, the complex geometry of the double helix DNA can be described by discrete finite element with few geometrical limitations. The two complementary sugar-phosphate back bones of dsDNA will be modeled as continuum double-helix curved beams. Furthermore, the interaction between complementary bases, such as hydrogen bond, can be treated as the equivalent beams. Also, due to the fact that the base-stacking interactions play a significant role in the stabilization of the DNA double helix, the van der Waals force between adjacent base pairs have evolved as the equivalent Lennard-Jones potential spring (equivalent L-J potential spring). Additionally, the simulation result of the proposed dsDNA finite element model can be accomplished by the commercial transient finite element code within affordable CPU time. Through the proposed dsDNA model, the dynamic structural transition of nicked dsDNA under external force/torque can be completely revealed. Moreover, the non-linear mechanical behavior and cooperative extensibility of dsDNA can be comprehensively understood.

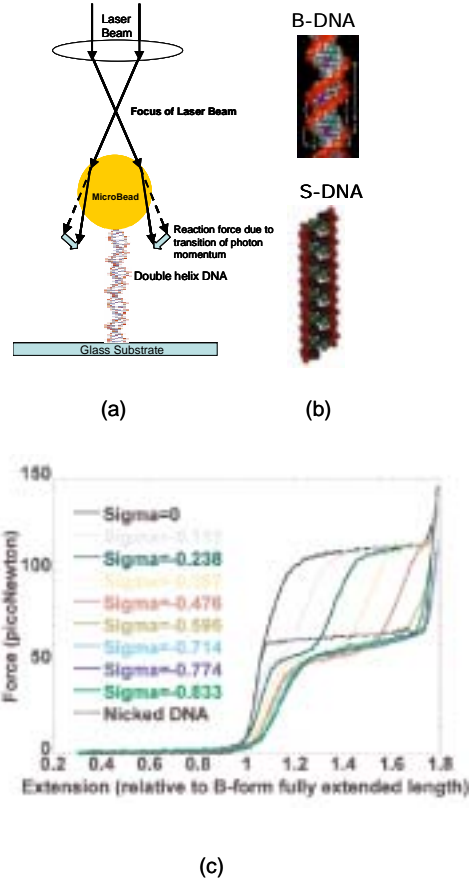


Figure 2: Schematic illustration of dsDNA single molecular experiment.

Transient Finite Element Model for dsDNA

■ Finite Element Theory

Using the principle of minimum potential energy, one can generate the equations for a constant-strain finite element. For each specific time ($t = t_i$), the total potential energy is a function of the nodal displacements $X(x, y, z)$ such that $\pi_p = \pi_p(X)$. Here the total potential energy is given by

$$\pi_p \Big|_{t=t_i} = U + \Omega_p \Big|_{t=t_i} \quad (1)$$

where U and Ω_p represent strain energy and energy of external loading, respectively. The above equation can be rewritten as a finite element integrated form[9]

$$\pi_p \Big|_{t=t_i} = \frac{1}{2} \iiint_V \left[\rho \{d\}^T [N]^T [N] \{d\} dV + \{d\}^T [B]^T [D] [B] \{d\} \right] dV - \left[\{d\}^T \{P\} \Big|_{t=t_i} + \iint_S \{d\}^T [N_s]^T [T_s] \Big|_{t=t_i} dS \right] \quad (2)$$

where $\{d\}$ represents the nodal vector, $\{\ddot{d}\}$ represents the nodal acceleration, ρ represents the density, $[B]$ is the strain-displacement matrix, $[D]$ is modulus of elasticity matrix, $[N]$ is the shape function matrix, $\{P\}$ is the external load vector and $[T_s]$ is the traction force matrix. The minimization of total potential energy with respect to each nodal displacement requires that

$$\left. \frac{\partial \pi_p}{\partial \{d\}} \right|_{t=t_i} = \left(\iiint_V [\rho][N]^T [N] \{\ddot{d}\} + [B]^T [D][B] dV \{d\} \right) \Big|_{t=t_i} - \left[\{P\} + \iint_S [N_s]^T [T_s] dS \right] = 0$$

namely,

$$\begin{aligned} \text{at } t = t_i, \quad & \left(\iiint_V [B]^T [D][B] dV \{d\} + \left(\iiint_V \rho [N]^T [N] dV \right) \{\ddot{d}\} \right) \\ & = \{P\} + \iint_S [N_s]^T [T_s] dS \end{aligned} \quad (3)$$

Finally, solving the linear system shown in Eq.(3) at each specific time, one can obtain the $\{d\}$ and the global nodal vector can be revealed.

Equivalent Theory of Meso-mechanics

Since the meso-mechanics of dsDNA comprises both quantum mechanics and continuum mechanics, a feasible equivalent theory should be established, capable of including the chemical bond forces in the global analysis of the dsDNA finite element model. The hydrogen bond force, which is the interaction between complementary bases, could mechanically transverse both moment and force, because there are at least two hydrogen bonds in the complement bases. Accordingly, the hydrogen bond force will be treated as the equivalent beam elements in the dsDNA finite element model.

Furthermore, the base-stacking interactions originate from the weak van der Waals attraction between the polar groups in the adjacent base pairs. Such interactions are short range, and their total effect is usually described by a potential of Lennard-Jones from (6-12 potential form [10]). Base-stacking interactions play a significant role in the stabilization of the DNA double helix. By the Crotti-Engesser theorem, one can obtain the L-J potential force versus displacement relationship:

$$\begin{aligned} f_{LJ} = & \frac{12AU_0}{l_0} \left(\frac{h_0 + \Delta l \cos \varphi_0}{h_0 + \Delta l} \right)^7 \left[1 - \left(\frac{h_0 + \Delta l \cos \varphi_0}{h_0 + \Delta l} \right)^6 \right] \\ & \left[\frac{h_0 (1 - \cos \varphi_0)}{h_0 \tan \varphi_0 (h_0 + \Delta l \cos \varphi_0)} \right] \end{aligned} \quad (4)$$

where f_{LJ} represents the stacking force, U_0 represents the base stacking intensity and Δl represents the distance between the adjacent base pairs. l_0 , h_0 and φ_0 represent the initial specific length, base pair height and folding angle of the dsDNA, respectively. Using Eq. (4), the non-linear mechanical properties of the equivalent L-J potential spring can be practicably established.

■ dsDNA Finite Element Model

To fully understand the dsDNA mechanical behavior, we will establish the proposed finite element model in this section. Due to that the classic B-DNA is stable in physiological aqueous solution, its geometrical structure has been chosen as the initial state of the said model, and the Writhe number of proposed dsDNA model has been assumed as zero. Moreover, both the major/minor groove and the sequence of the dsDNA were neglected for the sake of simplifying the proposed finite element model. Besides the equivalent hydrogen bond beam elements and equivalent base-stacking spring elements, the two complementary sugar-phosphate backbones of dsDNA will be modeled as continuum double-helix curved beams with geometrical nonlinear capability because the backbones would inherit the axial stress, bending moment and torque during stretching dsDNA. Additionally, the single base pair has been considered as a rigid rod, and the deformation of the base pairs are neglected.

The finite element model of dsDNA is then conducted, as shown in Figure 3. The figure 3, (a) represents the dsDNA with 147 bps (base pairs). (b) is the detail structure of (a), where the red circular double helices represent the sugar-phosphate chains and the blue rods represent the base pairs. Additionally, the yellow line and the green line in (c) represent the equivalent hydrogen bond beam type element and equivalent base-stacking spring element, respectively. Moreover, the non-linear spring constants of the equivalent L-J spring can be obtained from Eq. (4) with the folding angle equaling 55° . This model comprises 147 base pairs, and the initial length of the dsDNA approximately equals 50nm. In the nicked dsDNA simulation, one end of the backbone is mechanically fixed and another end is applied the external force, which is strictly proportioned to the time in the simulation.

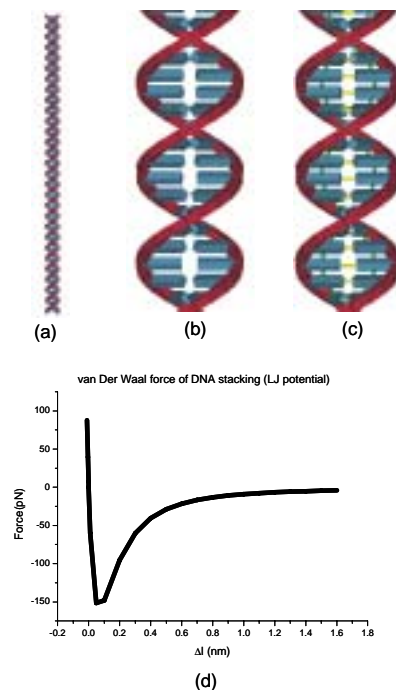


Figure 3: Finite element model of dsDNA.

Simulation Result of Nicked dsDNA Structural Transition

The dsDNA finite element model consists of 2,213 beam elements and 292 discrete spring elements, and is comprised of 4,281 nodes. The transient finite element model has been solved by commercial finite element analysis code LS-DYNA® (version 970) with the a CPU time of 20,652 seconds on IBM® SP2 SMP hardware.

The finite element simulation results of stretching nicked dsDNA revealed a continuous structural transition, which can be characterized by the three main stage of stretching the nicked dsDNA (Fig. 4). We will discuss the mechanical characteristics of these three stages in the following section.

■ Stage 1: B-DNA

When the external force is first applied on the B-DNA, the base pairs and the hydrogen bond balance the mechanical equilibrium between the two complementary sugar-phosphate backbones of the dsDNA. In this stage, both the backbone and the equivalent base-stacking spring inherit uniform axial reactant forces. However, the torsional rigidity of the dsDNA backbones resists the twisting of the complementary base pairs. As a result the geometry of the dsDNA remains B-DNA in stage 1 without structural transitions.

■ Stage 2: B-DNA to S-DNA (B-S Transition)

As the external force increases, so does the van der Waals reactant force between the adjacent base pairs increase. Until the distance between adjacent base pairs exceeds the limitation, the base-stacking fails and the B-S transition occurs at approximately 65 pN of tension. Meanwhile, the torque of the dsDNA local structure overcomes the backbone torsional rigidity and begins to untwist the double helix of the complementary backbone. Due to the transient mechanical effect, the untwisting starts from the nearest base pair where the external force applied, and propagates along the rest of the dsDNA. As the rotation of backbone, the double helical B-DNA transits to ladder S-DNA.

■ Stage 3: S-DNA

After the dsDNA has fully transited to the ladder-type S-DNA, the rotation of the local sugar-phosphate backbone terminates. In Stage 3, the base pairs and the hydrogen bond balance the mechanical equilibrium between two complementary sugar-phosphate backbones of dsDNA. Due to the fact that the ultimate loading of backbone molecules is approximately 476pN [11], the dsDNA structure will be broken if the hydrogen bond between the complimentary base pairs fails and the dsDNA will then be unzipped and opened.

Conclusion

In this paper, a novel transient finite element method with equivalent mesh-mechanics has been applied in a dsDNA stretching simulation. The dsDNA complementary sugar-phosphate chains were modeled as continuum double-helix curved beams. In addition, the Hydrogen bond and base-stacking between bases were modeled as the equivalent beam elements and spring elements in the proposed model, respectively. The continuous dynamic structural transition of stretching nicked dsDNA was revealed in the finite element simulation results. Moreover, the structural transition was characterized as three main stages, and the mechanical behavior of

stretching dsDNA was thoroughly elucidated. Furthermore, the proposed finite element model was applied in the analysis and prediction of the biological interactions between DNA and other proteins/enzymes, such as DNA binding protein or RNA polymerase.

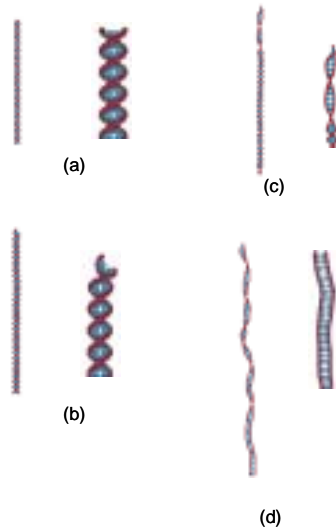


Figure 4: Structural transition of dsDNA. The left side figure represents the total dsDNA with 147 bps, and the right side figure represents the detail structure of left side dsDNA. (a) represents the initial condition of B-DNA. (b). (c) and (d) represent stage 1, stage 2 and stage 3, respectively.

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