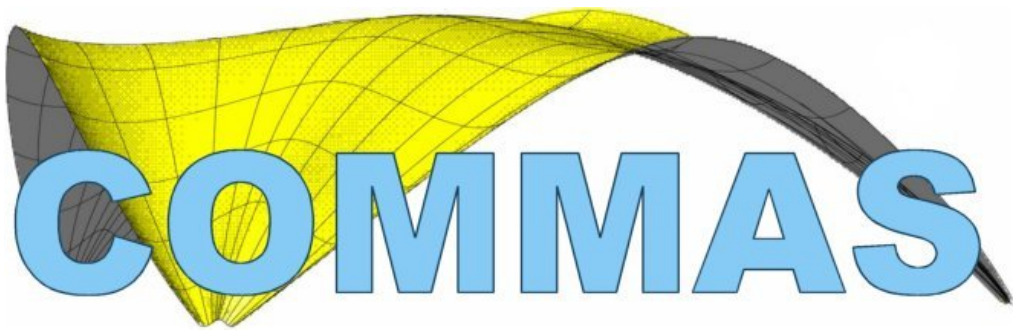
State and Future Perspectives in Computational Mechanics of Materials and Structures

Michael Ortiz, Caltech



Graduation Ceremony

Universität Stuttgart, June 13, 2003

COMMAS - Graduation

Congratulations! to the students and to the faculty

COMMAS - Graduation

- **Core Courses**
  - Engineering Materials
  - Discretization Methods
  - Software Development
  - Structural Dynamics
  - Computational Mechanics of Materials
  - Computational Mechanics of Structures
  - Continuum Mechanics
  - Advanced Materials and Smart Structures

"Graduates of this unique Master Programme will be qualified to find employment in a wide range of professions, e.g. as research and development engineer or technical advising manager in industry, at laboratories or universities."

COMMAS - Graduation

- **Faculty:**
  - ***Prof. Dr. rer. nat. Hans-Joachim Bungartz***
  - ***Prof. Dr.-Ing. Peter Eberhard***
  - ***Prof. Dr.-Ing. Wolfgang Ehlers***
  - ***Prof. Dr.-Ing. Rolf Eligehausen***
  - ***Prof. Dr.-Ing. Lothar Gaul***
  - ***Prof. Dr.-Ing. Bernd H. Kröplin***
  - ***Prof. Dr.-Ing. Christian Miehe***
  - ***Prof. Dr.-Ing. Ekkehard Ramm***
  - ***Prof. Dr.-Ing. Hans-W. Reinhardt***
  - ***Prof. Dr. rer. nat. Siegfried Schmauder***
  - ***Prof. Dr.-Ing. Pieter A. Vermeer***

COMMAS - Graduation

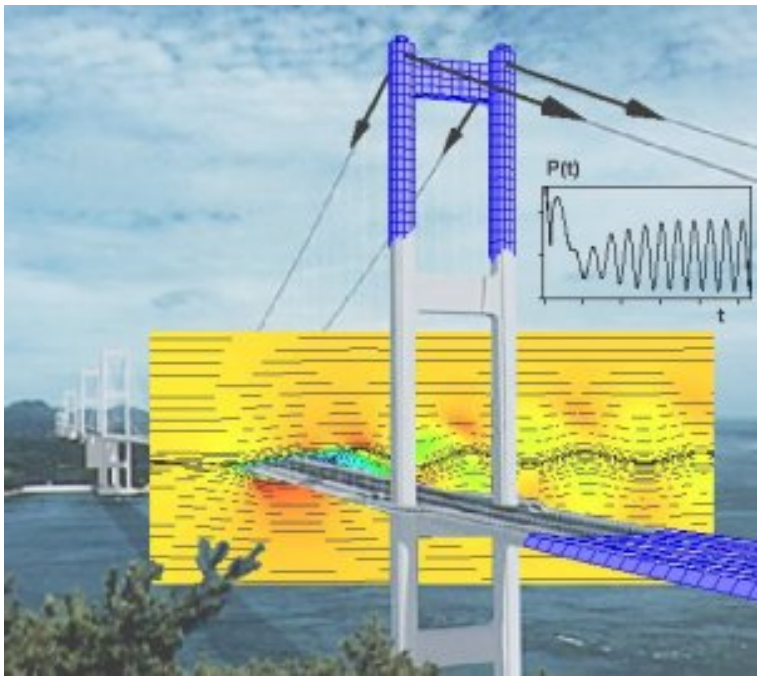
- **Faculty:**
  - ***Prof. Dr. rer. nat. Hans-Joachim Bungartz***
  - ***Prof. Dr.-Ing. Peter Eberhard***
  - ***Prof. Dr.-Ing. Wolfgang Ehlers***
  - ***Prof. Dr.-Ing. Rolf Eligehausen***
  - ***Prof. Dr.-Ing. Lothar Gaul***
  - ***Prof. Dr.-Ing. Bernd H. Kröplin***
  - ***Prof. Dr.-Ing. Christian Miehe***
  - ***Prof. Dr.-Ing. Ekkehard Ramm***
  - ***Prof. Dr.-Ing. Hans-W. Reinhardt***
  - ***Prof. Dr. rer. nat. Siegfried Schmauder***
  - ***Prof. Dr.-Ing. Pieter A. Vermeer***

COMMAS - Scope

What can we compute?

(almost) everything!

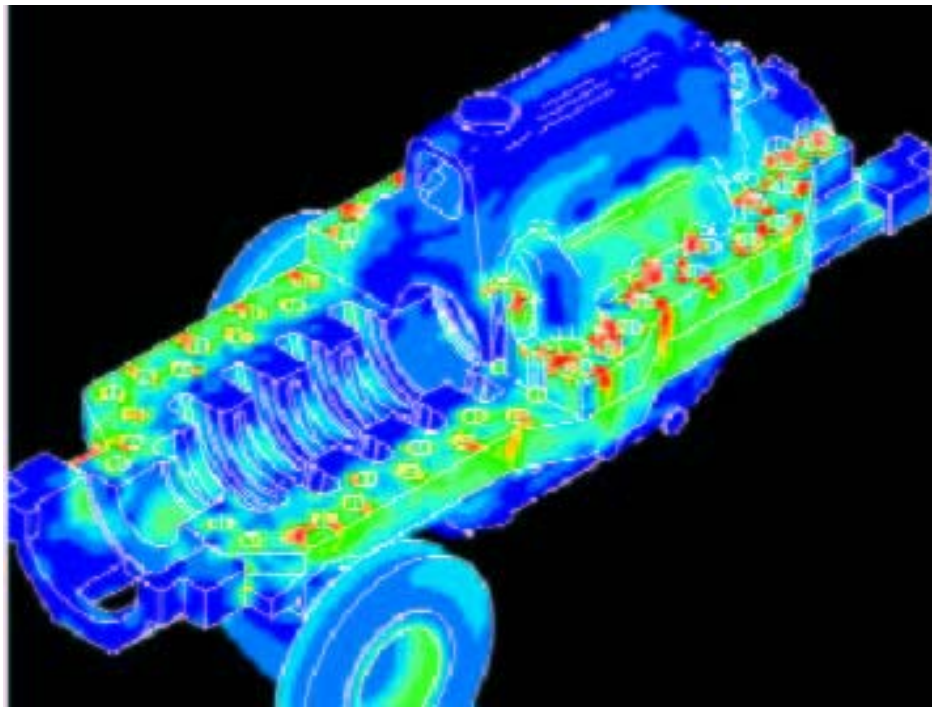
COMMAS – Structural mechanics



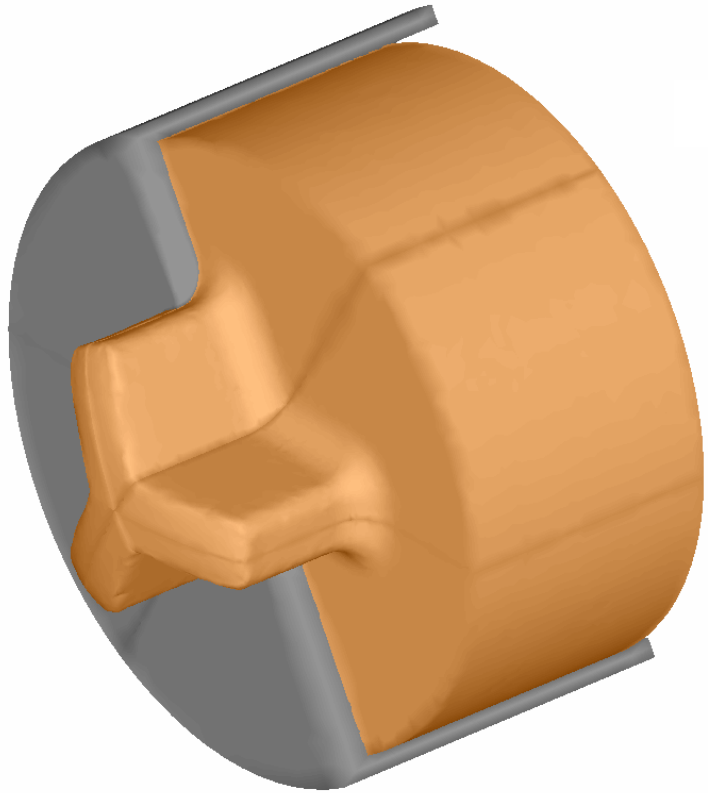
- Analysis and design of engineering structures
- Geotechnical engineering
- Earthquake engineering

M Ortiz
06/11/03

COMMAS – Design & manufacturing



ABAQUS, Inc

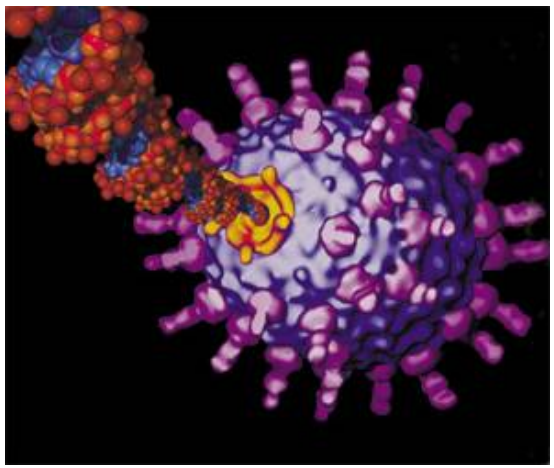


Vallellano and Ortiz (2000)

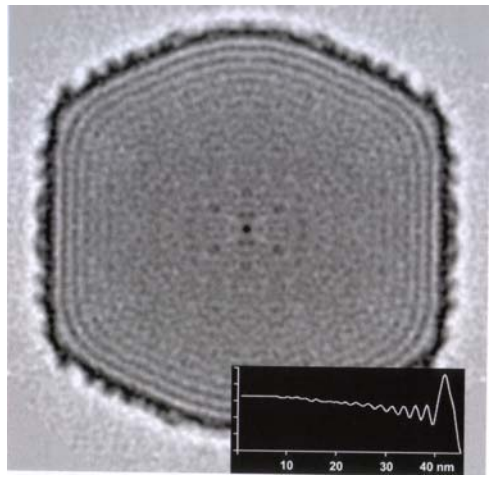
- Early evaluation of concepts
- Complex design analysis and development
- Process simulation and optimization

COMMAS applications - Biomechanics

Viral DNA encapsidation



ø29 bacteriophage
Nature, **408** (2000)



Encapsidated T4 genome
(Olson et al., 2001)

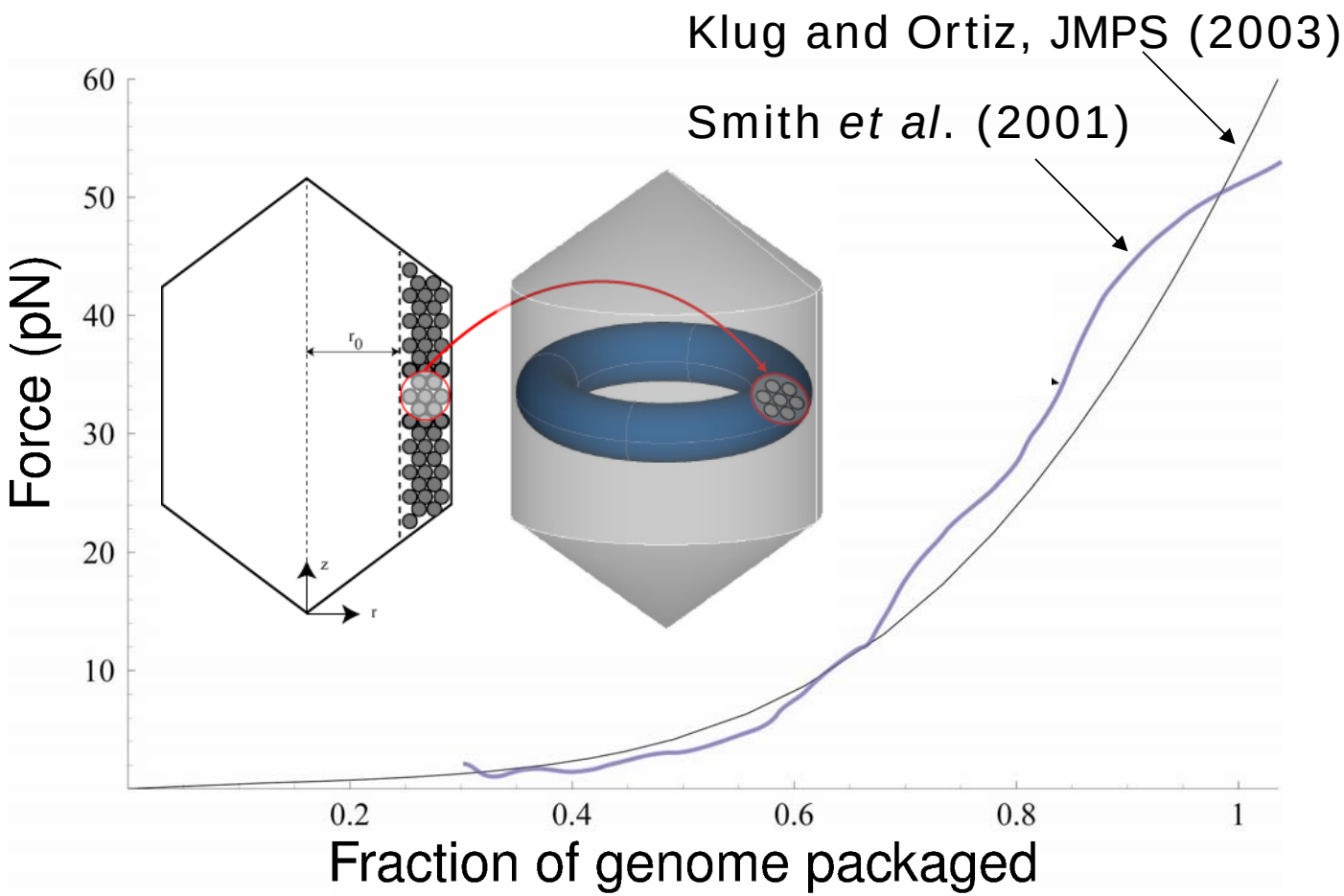
$D \approx 9''$

$L \approx 810'$

M Ortiz
06/11/03

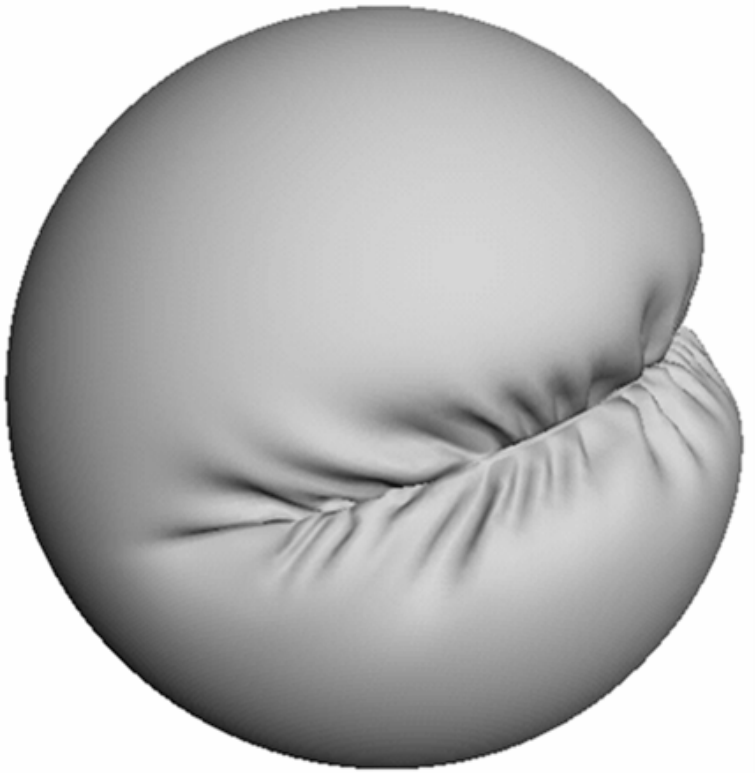
COMMAS applications - Biomechanics

Viral DNA encapsidation

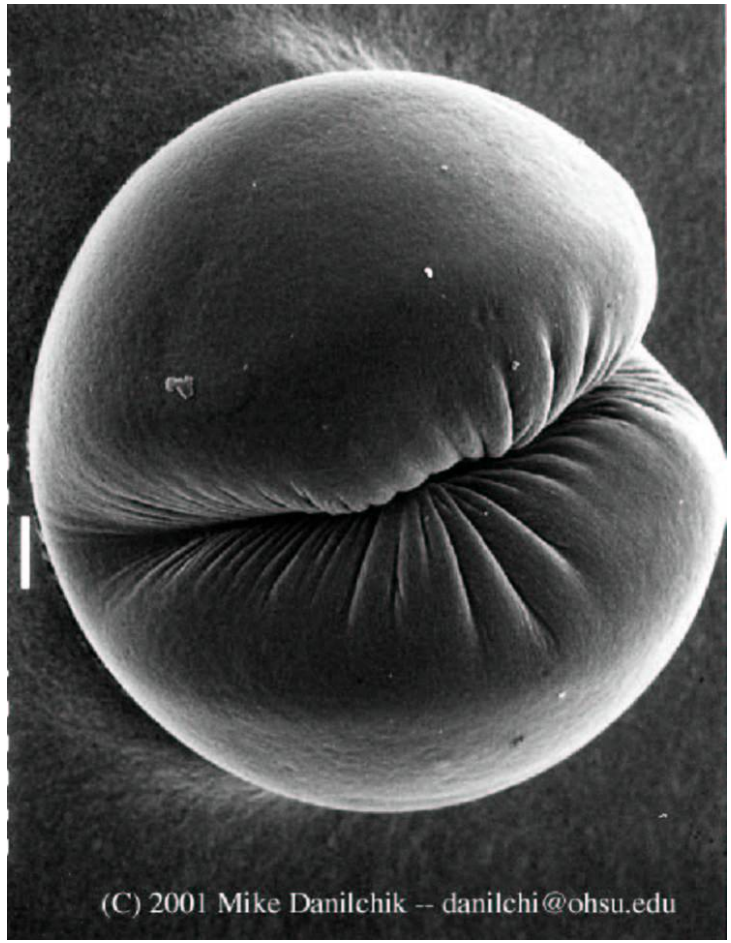


M Ortiz
06/11/03

COMMAS applications - Biomechanics



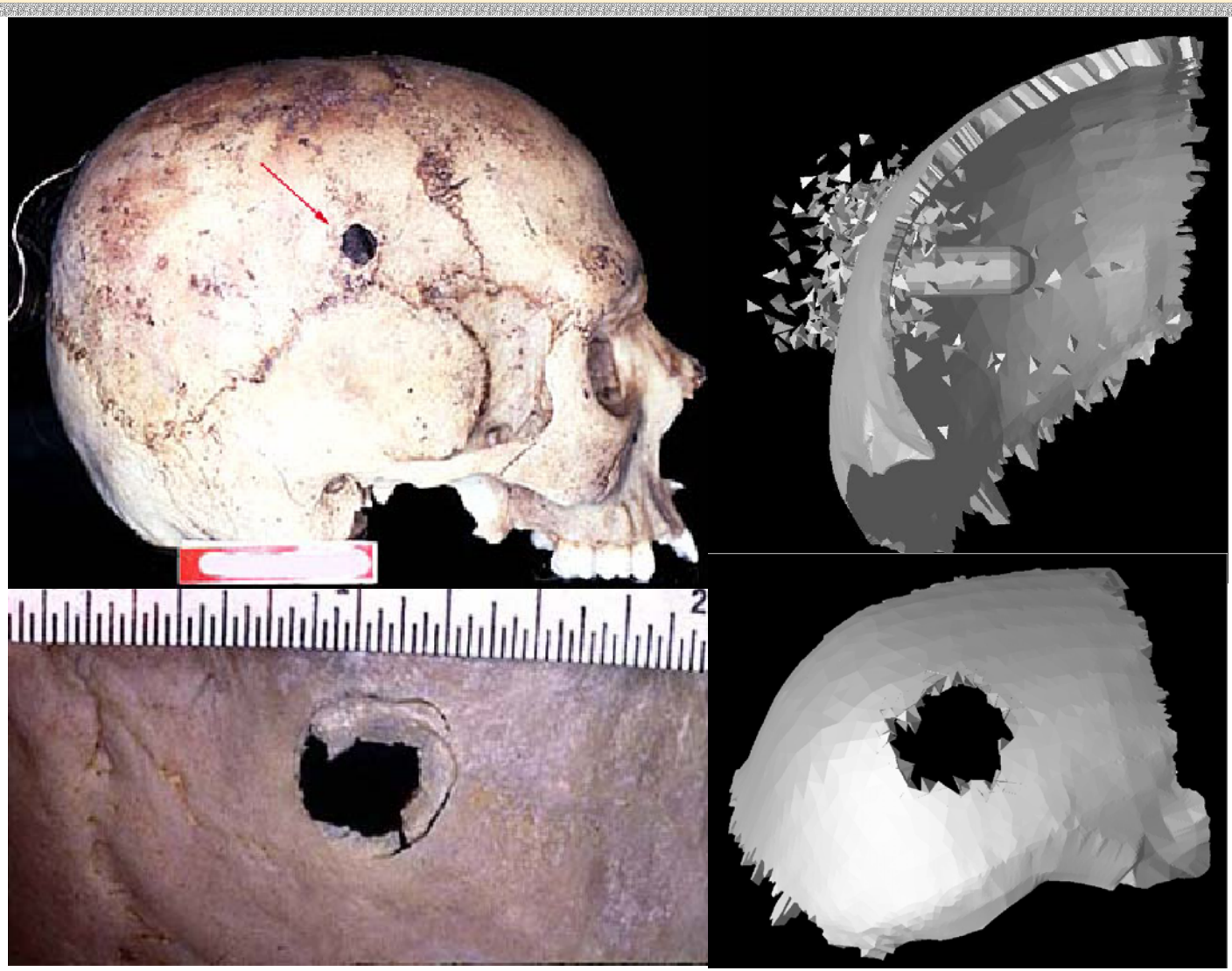
F. Cirak (2002)



Division of echinoid (sea-urchin) egg

M Ortiz
06/11/03

COMMAS applications - Biomechanics



Mota *et al*., JCM (2003)

M Ortiz
06/11/03

COMMAS applications - Space structures

First European Workshop on
Inflatable Space Structures

21-22 May 2002
ESTEC, Noordwijk,

The Netherlands

Organized by the
European Agency (ESA)
In collaboration with CNES,
ASI, Rosaviacosmos and DLR

M Ortiz
06/11/03

COMMAS applications - Space structures

- KIRTLAND AIR FORCE BASE, N.M. - Air Force Research Laboratory Space Vehicles Directorate engineers prepare inflatable membrane for testing in the Directorate's Structures and Controls Laboratory. Looking a lot like a giant contact lens, this experimental lightweight device may pave way for future, inexpensive weight-saving technologies that enable large space structures. (Air Force photo by Art Goodman)

Air Force Research Laboratory Public Affairs
Released 5 November, 1999

M Ortiz
06/11/03

COMMAS applications - Space structures

Schematic diagram (not to scale) of the 14-meter Inflatable Antenna Experiment (IAE) flown from the Space Shuttle.

Four views of the deployment. Two of the views are from the shuttle and two of the views are from the wide and narrow FOV cameras located on the IAE.

The IAE was a joint JPL, NASA/Goddard and L'Garde program

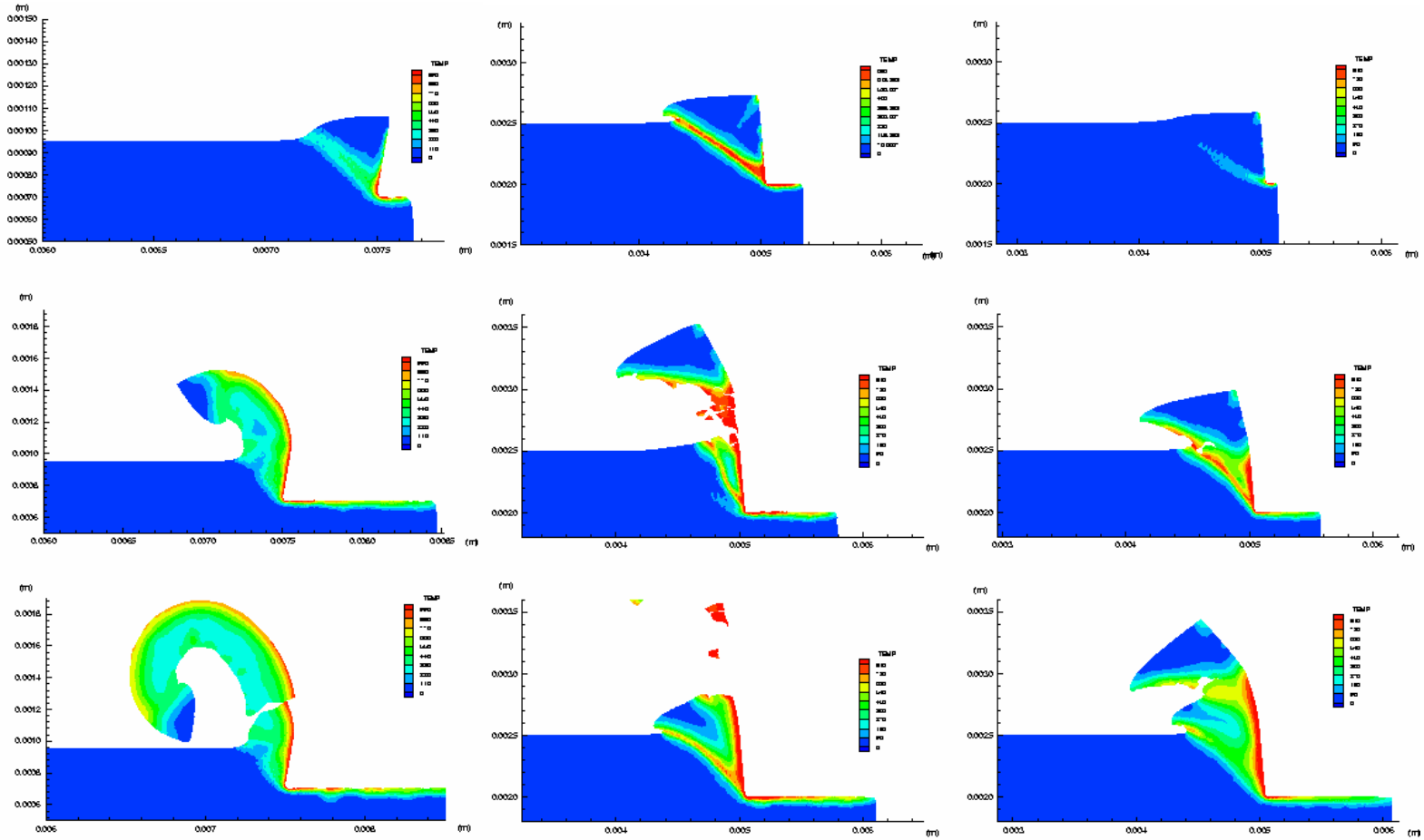
M Ortiz
06/11/03

Is what we compute any good?
The burden of proof: Validation...

M Ortiz
06/11/03

Validation - High-speed machining

High-speed machining – AISI 4340 steel



Cutting speed = 20 m/s | Cutting speed = 20 m/s | Cutting speed = 10 m/s

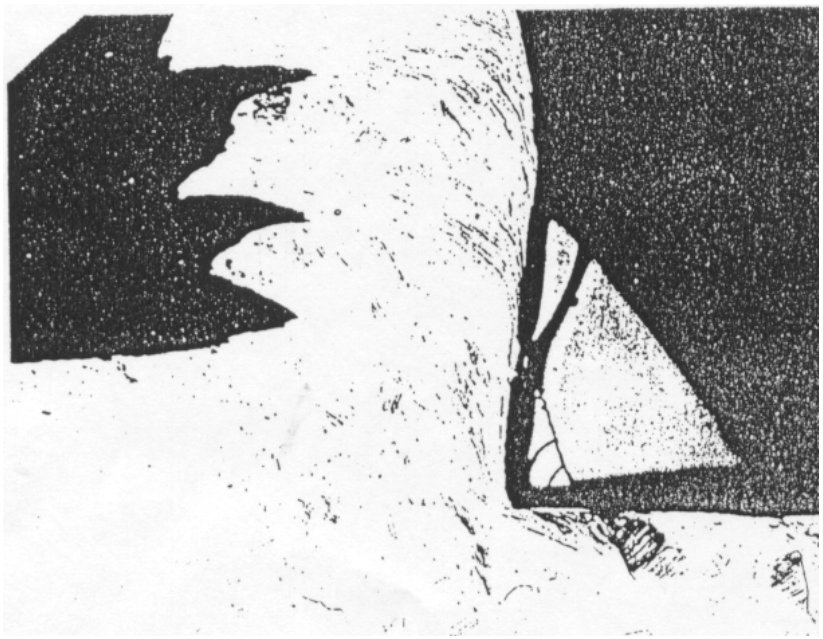
(Marusich and Ortiz, IJNME, 1995)

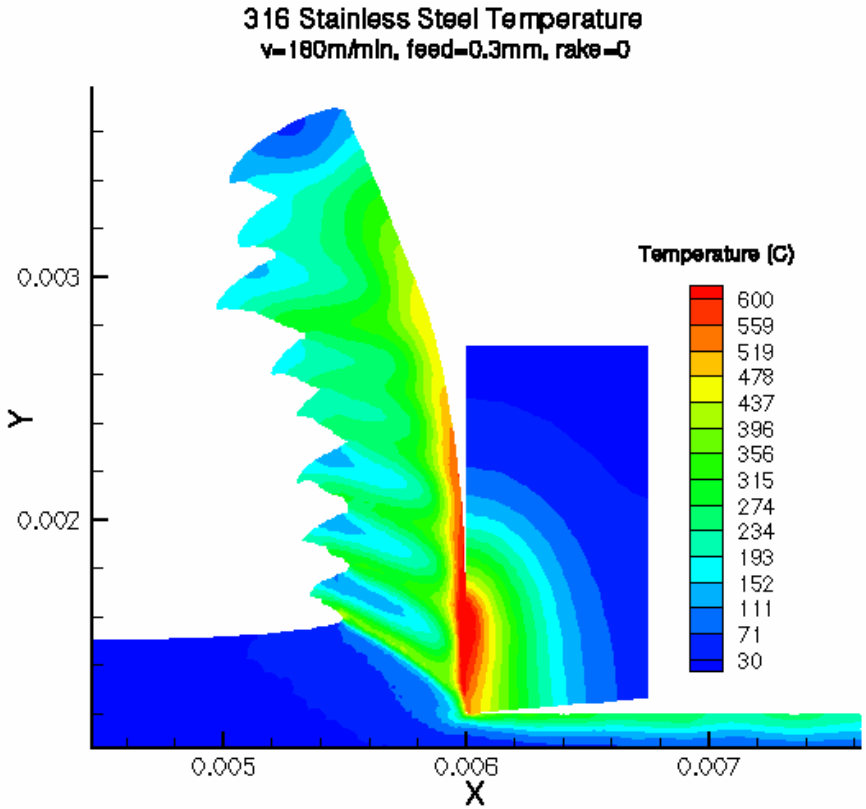
M Ortiz
06/11/03

Validation - High-speed machining

Chip Morphology Validation

316 Stainless Steel





Photomicrograph

Simulation

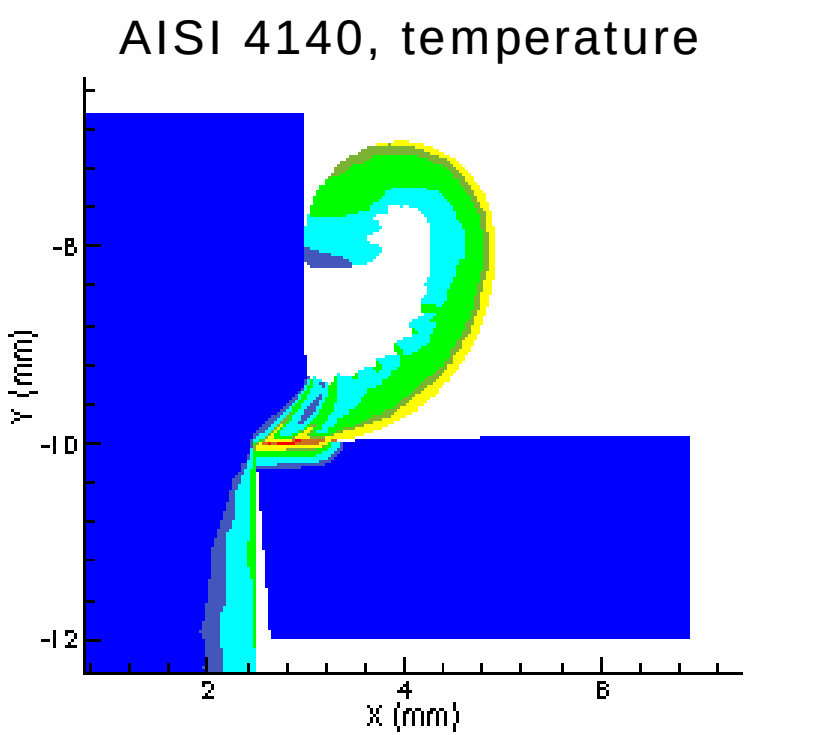
(Courtesy of Third Wave Systems Inc)

M Ortiz
06/11/03

Validation - High-speed machining

Chip Morphology Validation

High-speed photography
(Courtesy of Sandvik Coromant)



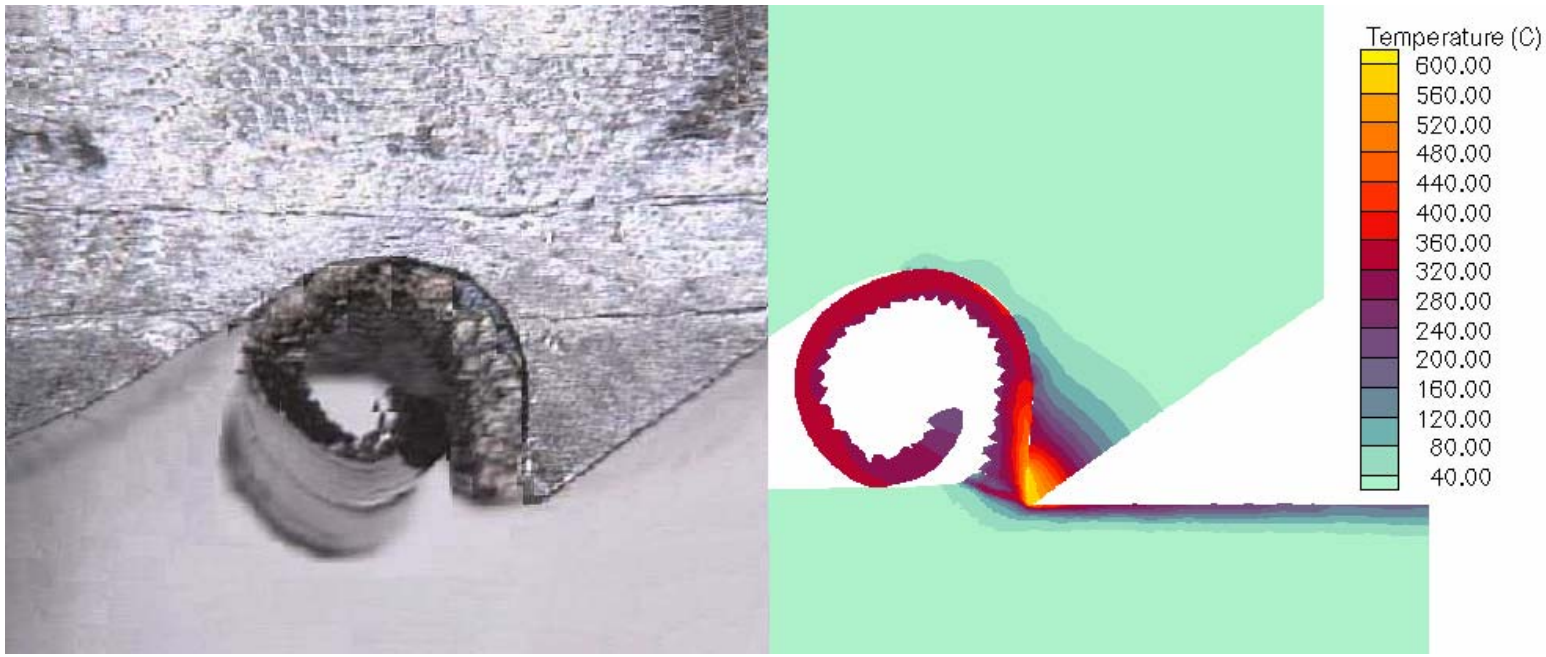
Simulation

(Courtesy of Third Wave Systems Inc)

M Ortiz
06/11/03

Validation - High-speed machining

Chip Morphology Validation



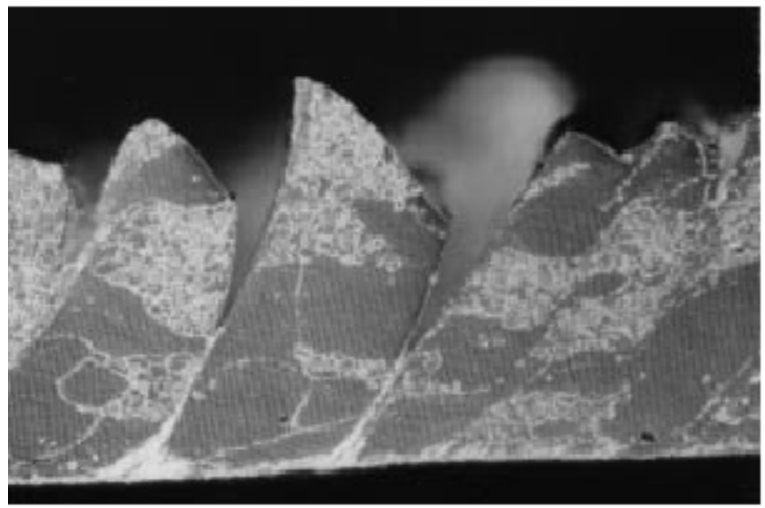
(Courtesy of IWH – Switzerland)

(Courtesy of Third Wave Systems Inc)

M Ortiz
06/11/03

Validation - High-speed machining

Chip Morphology Validation



(Courtesy of Boeing-Seattle)

Simulation

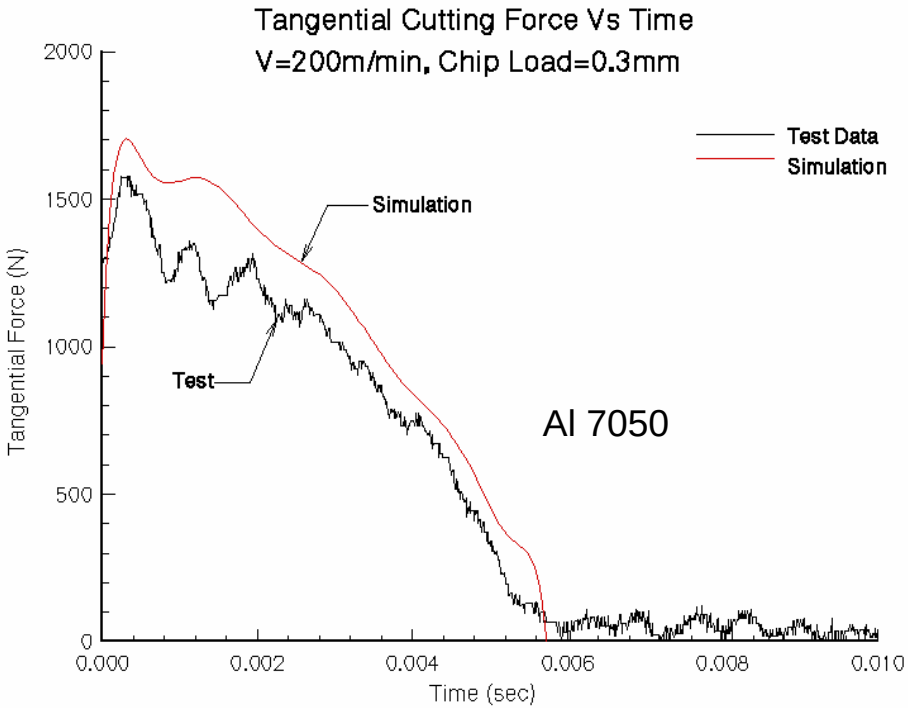
Machined Chip

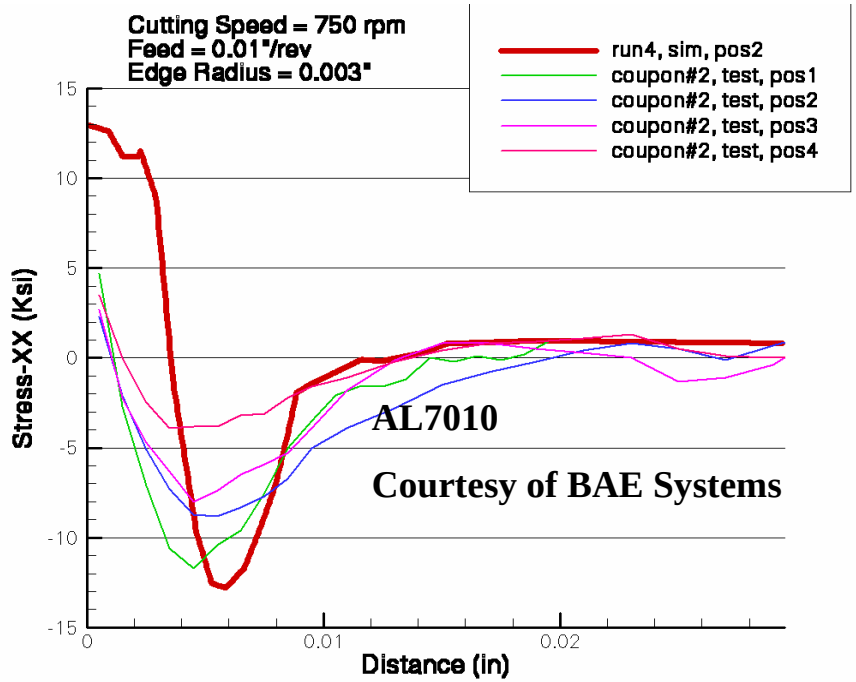
(Courtesy of Third Wave Systems Inc)

M Ortiz
06/11/03

Validation - High-speed machining

High-speed machining - Experimental validation





Cutting force validation

Residual Stress Validation

(Courtesy of Third Wave Systems Inc)

M Ortiz
06/11/03

COMMAS – Multiscale modeling

Calculations are only as good as the material model used (and never better)

COMMAS - Multiscale modeling

- Fidelity of simulation codes is critically limited by uncertainties in engineering (empirical) material models
- In order to reduce this uncertainty, we adopt a mechanistic viewpoint:
  - *Identify underlying unit mechanisms at lower lengthscales*
  - *Model each unit mechanism in turn*
  - *Compute effective behavior (averaging)*
- The recursive application of these steps leads to **Multiscale Modeling**:

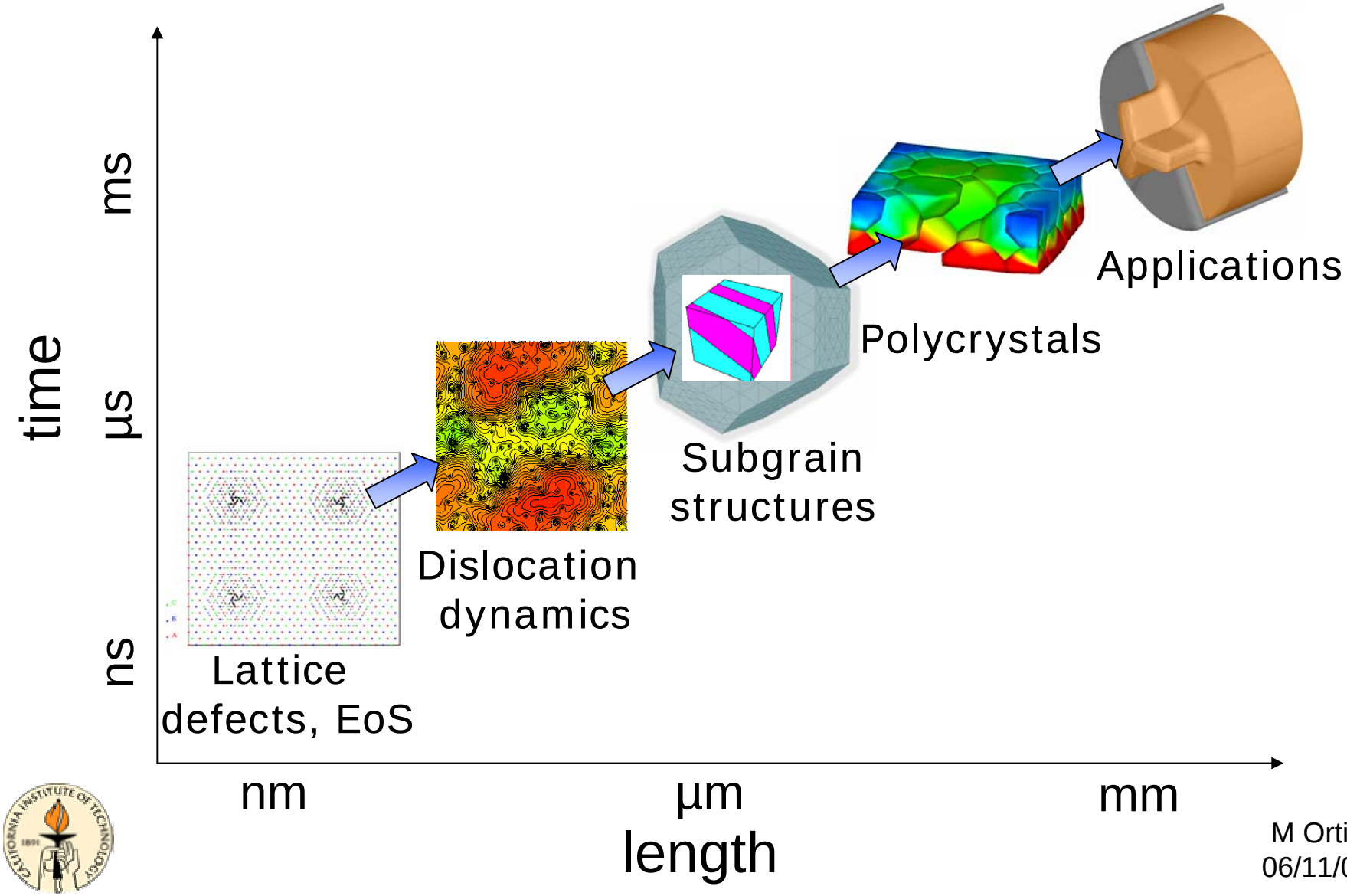
Quantum Chemistry → **Macroscale**

M Ortiz
06/11/03

COMMAS - Multiscale modeling

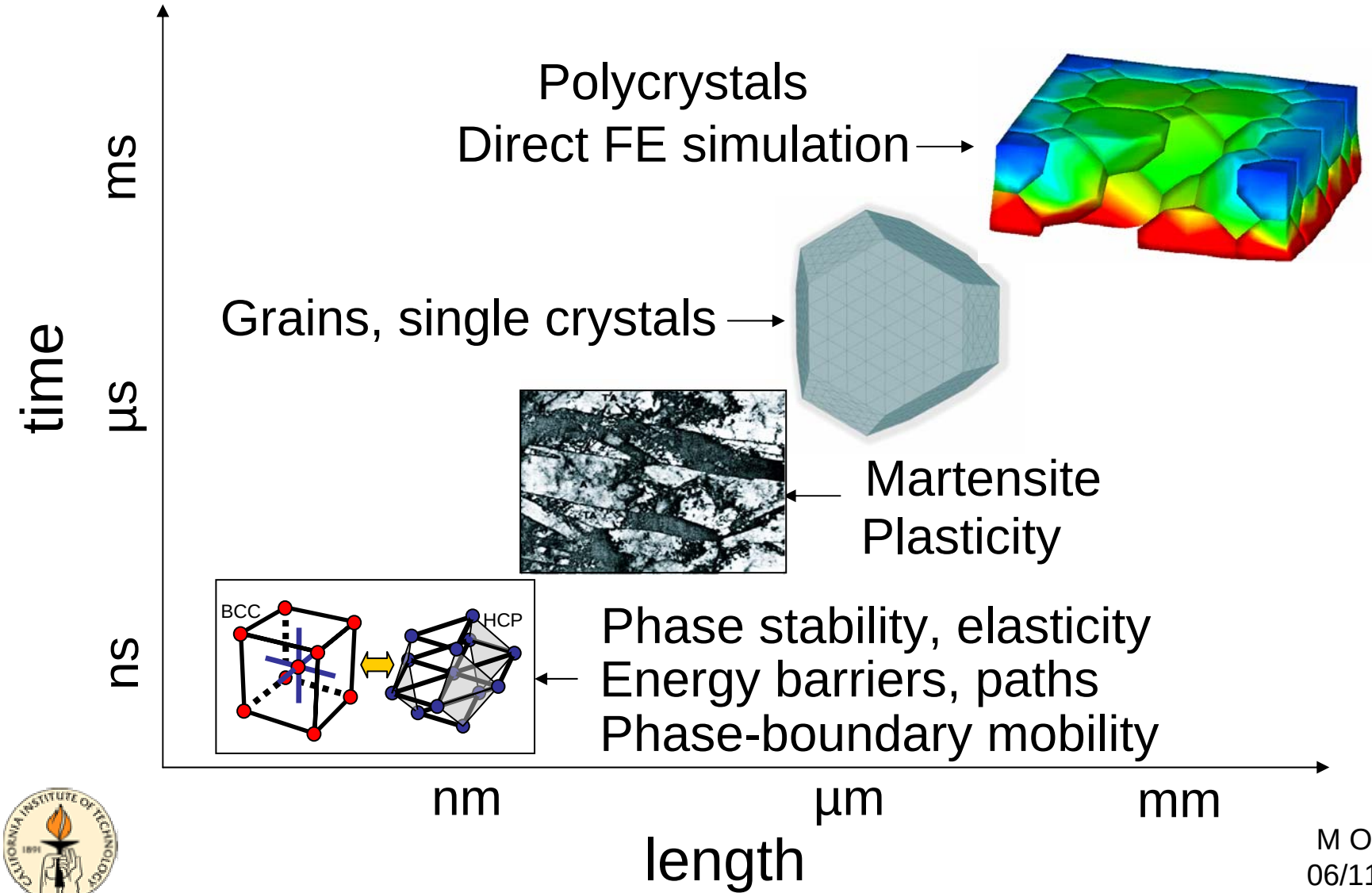
- Analysis:
  - *Homogeneization + relaxation*
  - *Statistical mechanics + renormalization group*
- Analytical methods give functional form of effective theory, but have trouble with
  - *Kinetics*
  - *Algorithmic implementation*
- Direct numerical simulation (MD, DD, PhF, FE...)
  - *Concurrent multiscale simulations*
  - *Calculation of material constants*
  - *Elucidation of mechanisms*
  - *Verification and validation*

Multiscale modeling – Metal plasticity



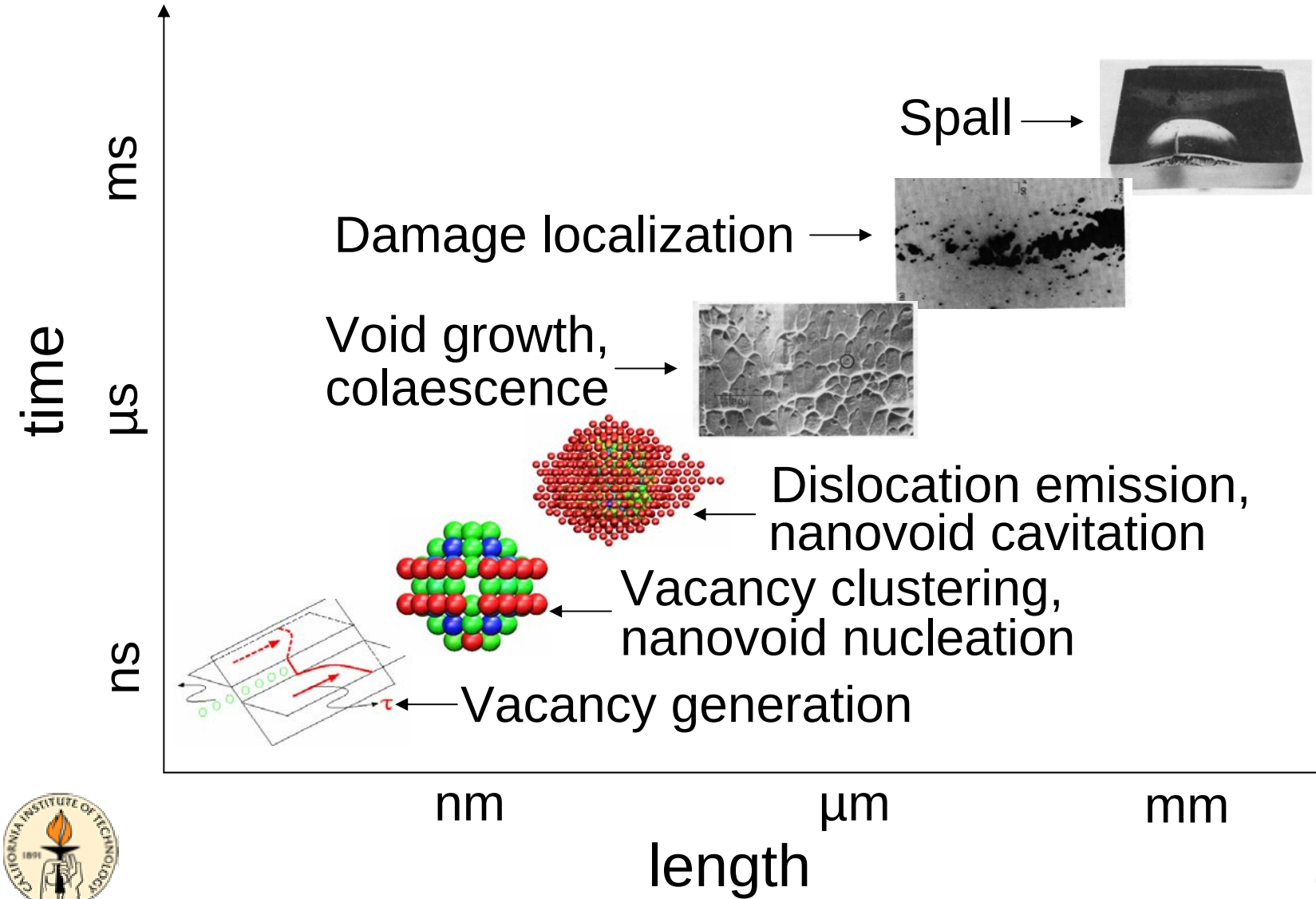
M Ortiz
06/11/03

Multiscale modeling - Martensite



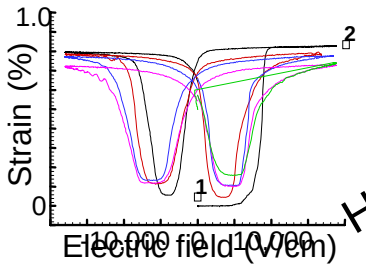
M Ortiz
06/11/03

Multiscale modeling - Spall



M Ortiz
06/11/03

Multiscale modeling – Active materials



Homogenization

Relaxation

10^{-8} -10^{-6} m

10^{-7} -10^{-4} m

10^{-6} m

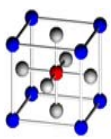
10^{-2} m

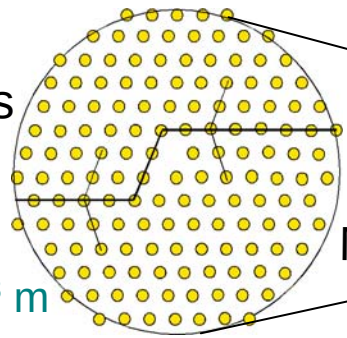
Validation of micropump predicted by theory

Quasicontinuum

Renormalizatio

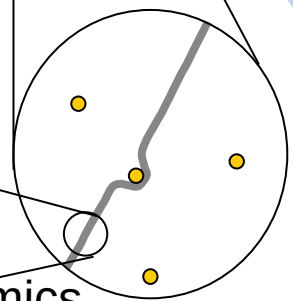
Quantum Mechanics





10^{-10} -10^{-8} m

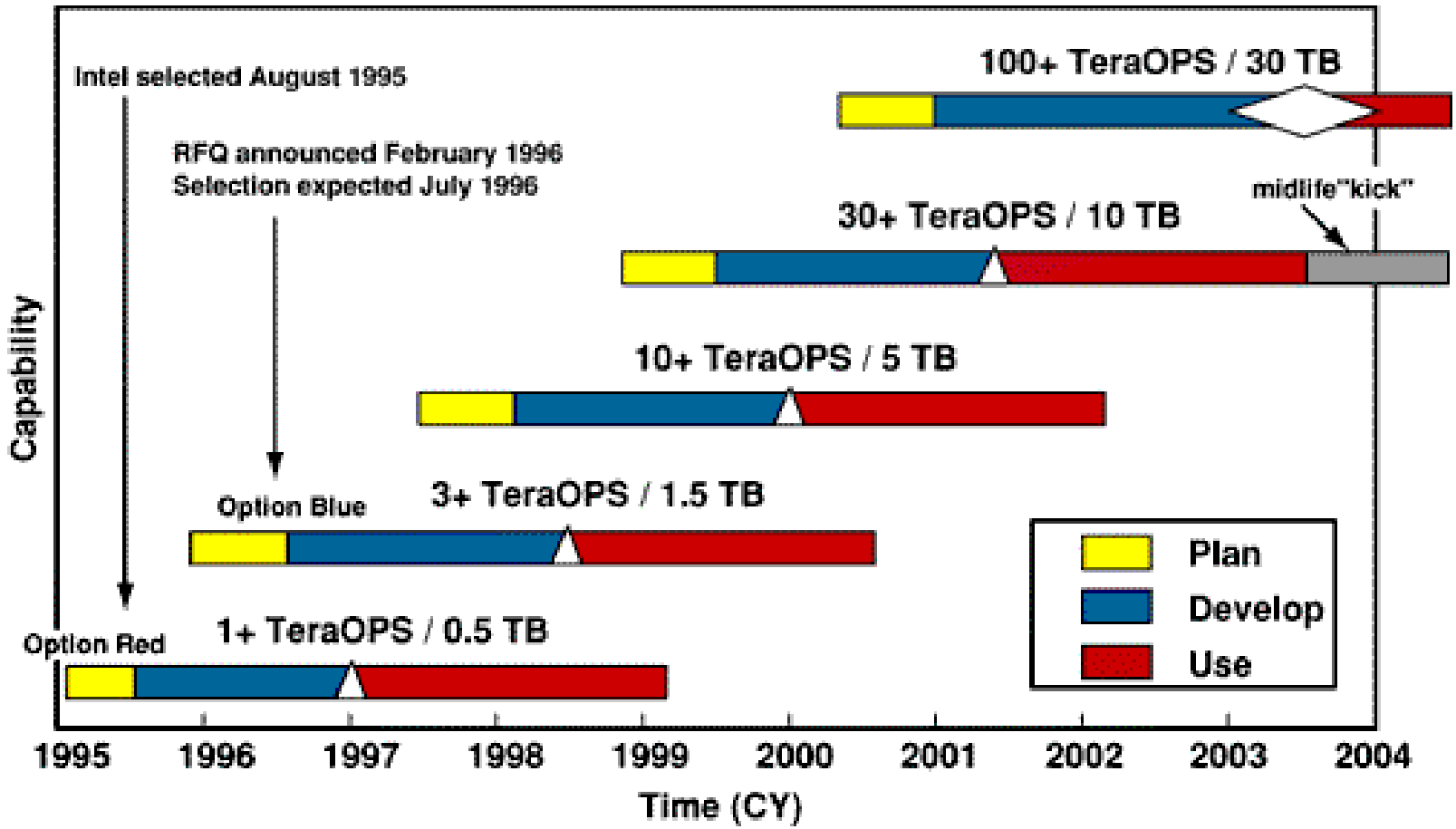
Molecular Dynamics



10^{-8} m

M Ortiz
06/11/03

Multsicale modeling - Platforms



ASCI computing systems roadmap

M Ortiz
06/11/03

COMMAS – Outlook

Is COMMAS a mature field? Hardly!

M Ortiz
06/11/03

COMMAS - Outlook

- Challenges abound:
  - *Automatic adaptive meshing*
  - *Interpolation of large deformations, incompressibility*
  - *Convergence analysis in:*
    - *Finite elasticity*
    - *Fragmentation*
    - *Shape optimization*
  - *Concurrent multiscale simulation*
  - *Microstructure evolution, kinetics*
  - *Material parameter identification*
  - *Symplectic, energy-momentum conserving time-stepping algorithms*
  - *Scalable parallel processing*

and many others...

COMMAS – Outlook

M Ortiz
06/11/03