SAND2007-5858C

The Application of Computational Methods for Materials Design

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Albuquerque, NM

MS&T 2007
Discovery and Optimization of Materials through Computational Design

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under the Contract DE-AC04-94AL-85000.

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An ~actual discussion that took place ~13 years ago.

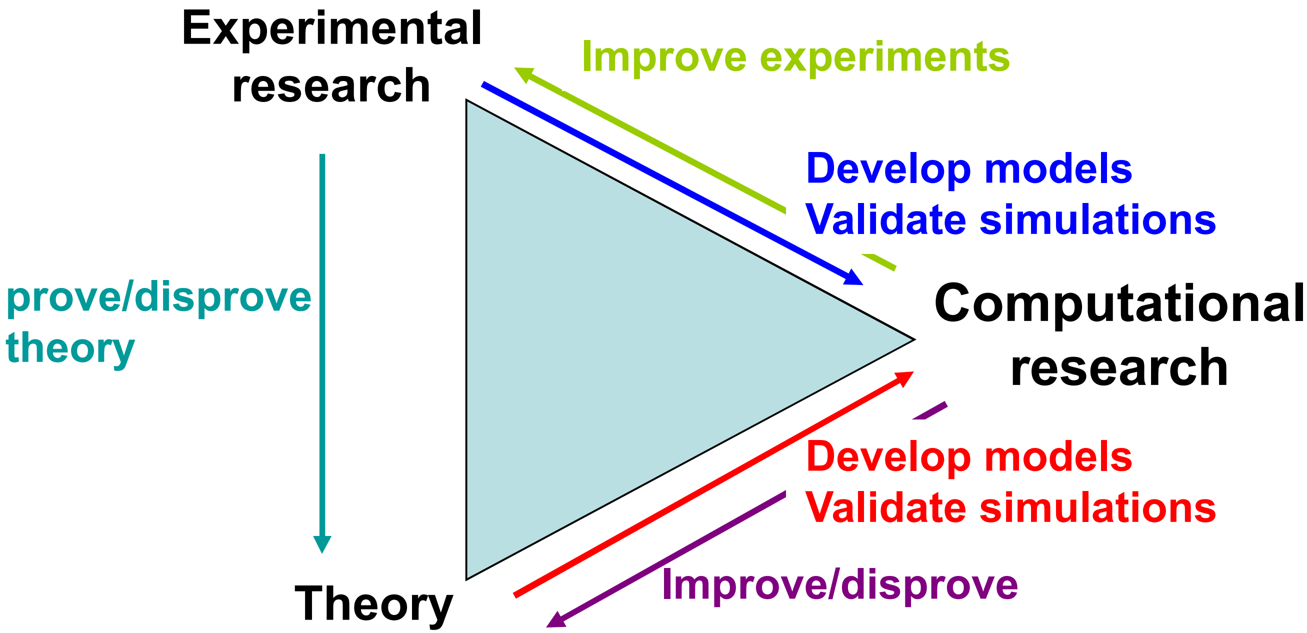
Computational Scientist	I can simulate simple, solid-state sintering.
Team leader	We can simulate solid-state sintering.
Manager	We have the capability to simulate sintering.
Executive	Why are we spending so much to experimentally determine sintering behavior? Eliminate the experiments!
Computational Scientist	Oh no! How did this happen? What did I say?

Invariably, it resulted in this consequence

Computational Scientist	I can simulate sintering of a totally pure, single phase, isotropic, idealized material with no inclusions. The results are non-dimensional in time and space. Although almost no technologically important material behaves this ideally, we can provide microstructural information and constitutive equations describing shrinkage that will help design a better product.
Team leader	How does simulating the idealized case help this team with the real material case?
Manager	What? If you can only simulate idealized material why do we do this at all. I will recommend we eliminate the computer simulations and increase funding for experiments
Computational Scientist	Oh no! How did this happen? What did I say?

Integrating computational research with experimental research and theory is necessary

Integration of computational research with experiments and theory results in a better answer.



Today's Issues

Computational Scientist	**I need these experiments to refine my model. How do I obtain the necessary resources?**
Design Engineer	**I cannot analyze this problem with this code because I don't know which model/BC/mesh/… to choose**
Funding Manager	**How much money/time will computer simulations save?**
Manager	**How do I allocate my computational resources to have maximum impact?**
Executive	**Widgits Inc. has been making widgits for 50 years, why should I develop computational capabilities to make widgits now?**

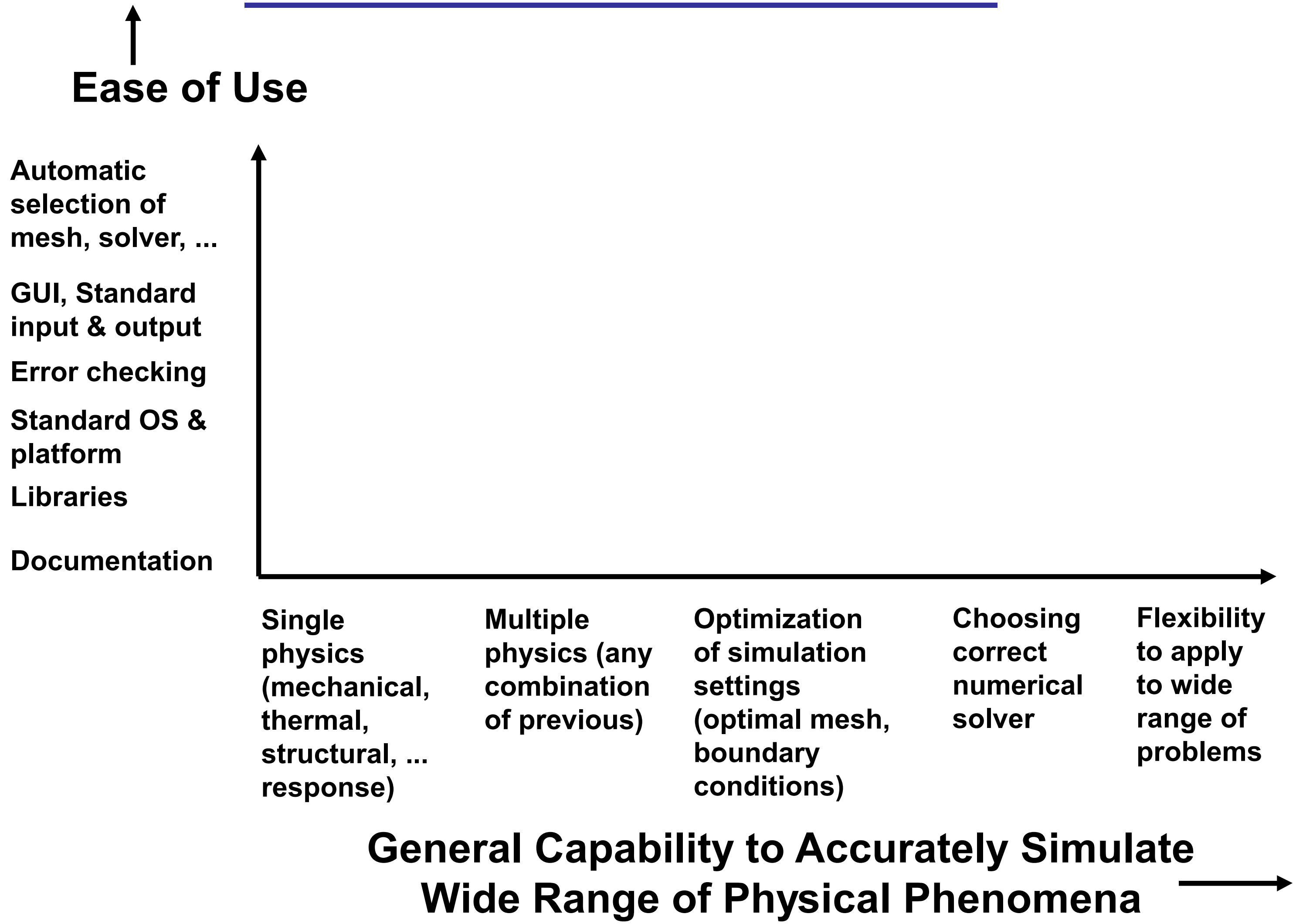
Objective

- Present a conceptual framework
  - Codes, Models, Algorithms, Solvers, …
  - How these relate to each other
  - Where does experimental research and theory fit in
- This framework may help answer questions like
  - Why integrate modeling and simulations into R&D?
  - How much do simulations cost?
  - How much *and which* experimental work is necessary

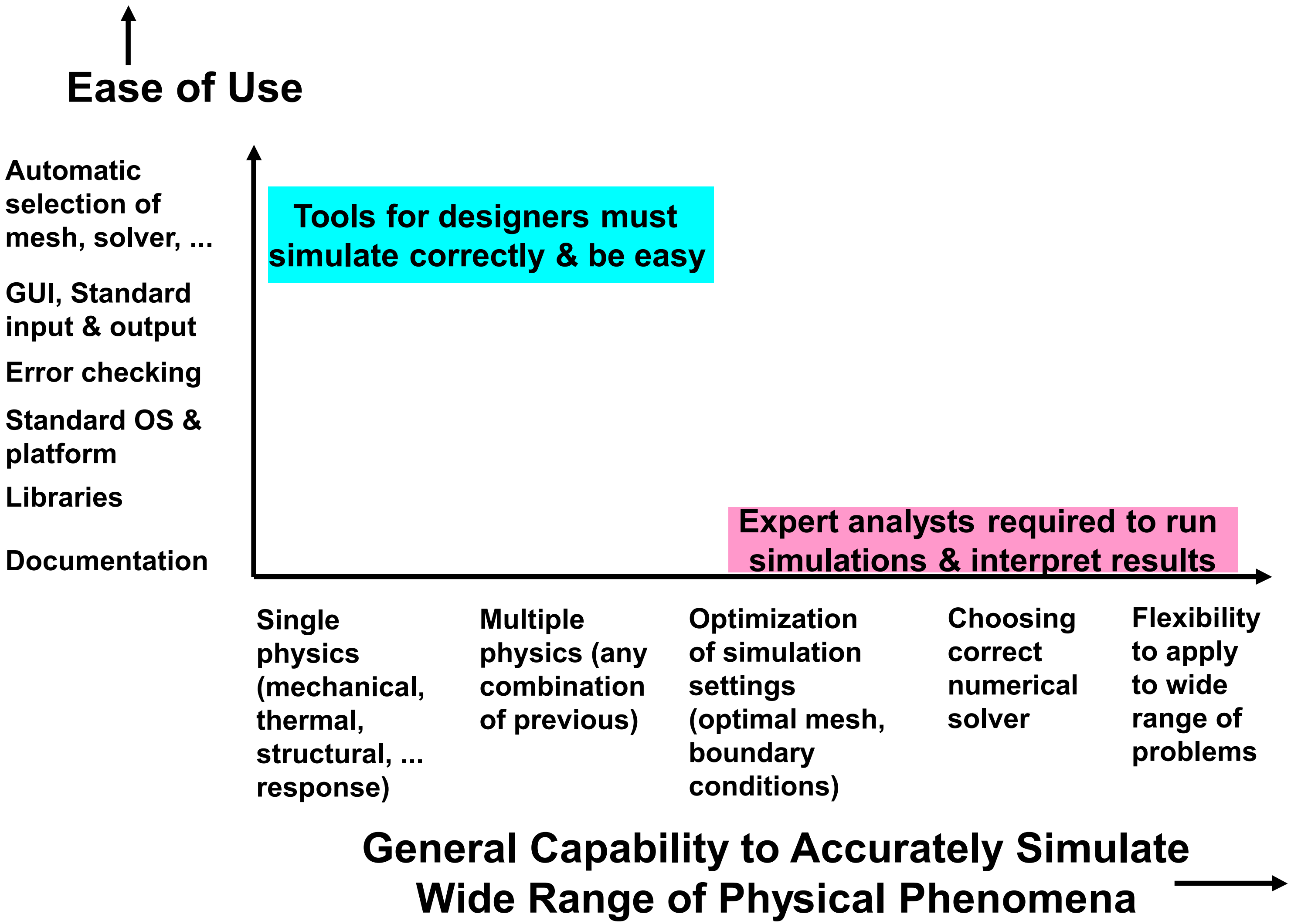
Single physics (mechanical, thermal, structural, ... response)	**Multiple physics (any combination of previous)**	**Optimization of simulation settings (optimal mesh, boundary conditions)**	**Choosing correct numerical solver**	**Flexibility to apply to wide range of problems**

General Capability to Accurately Simulate Wide Range of Physical Phenomena →

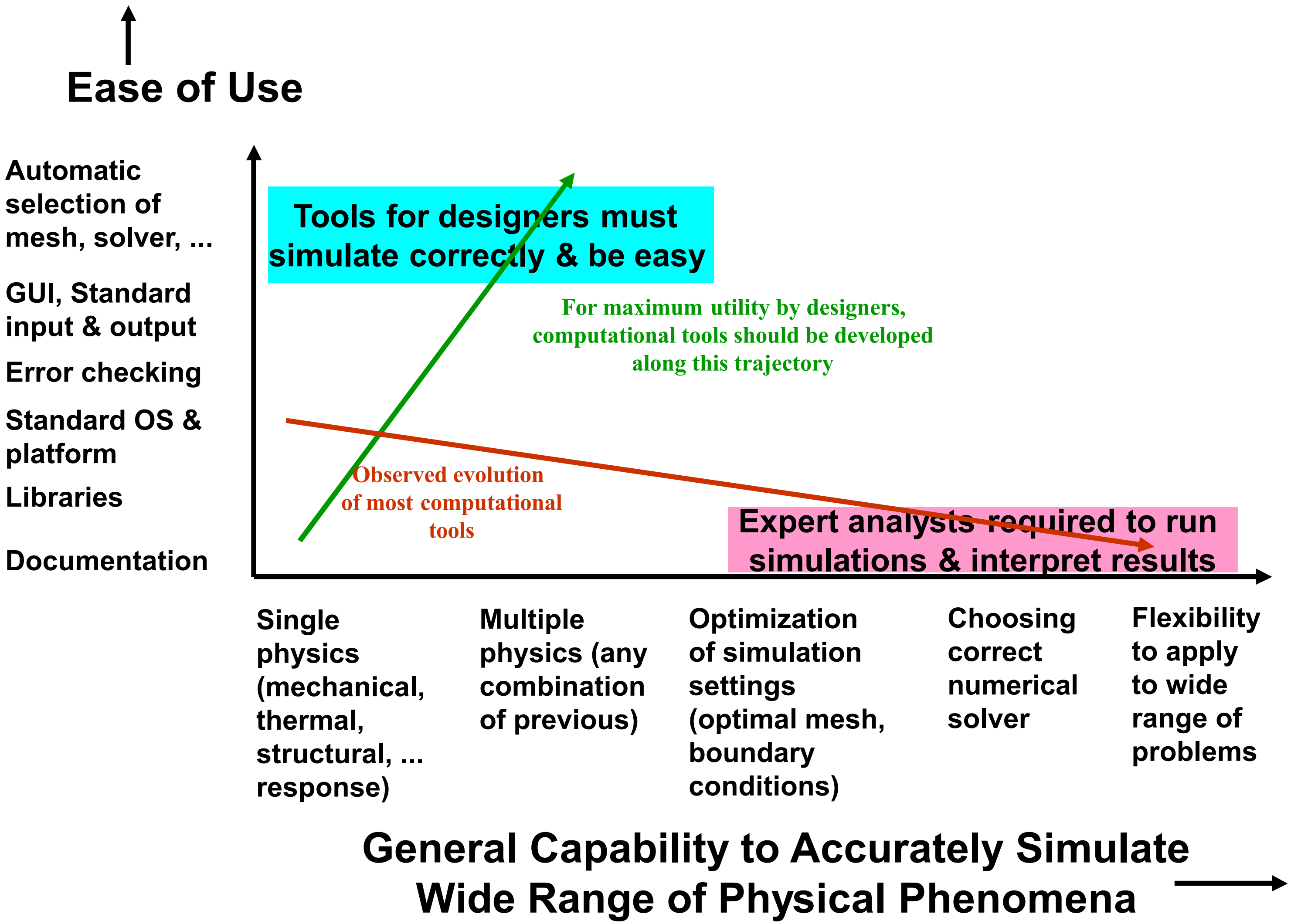
Conceptual Framework



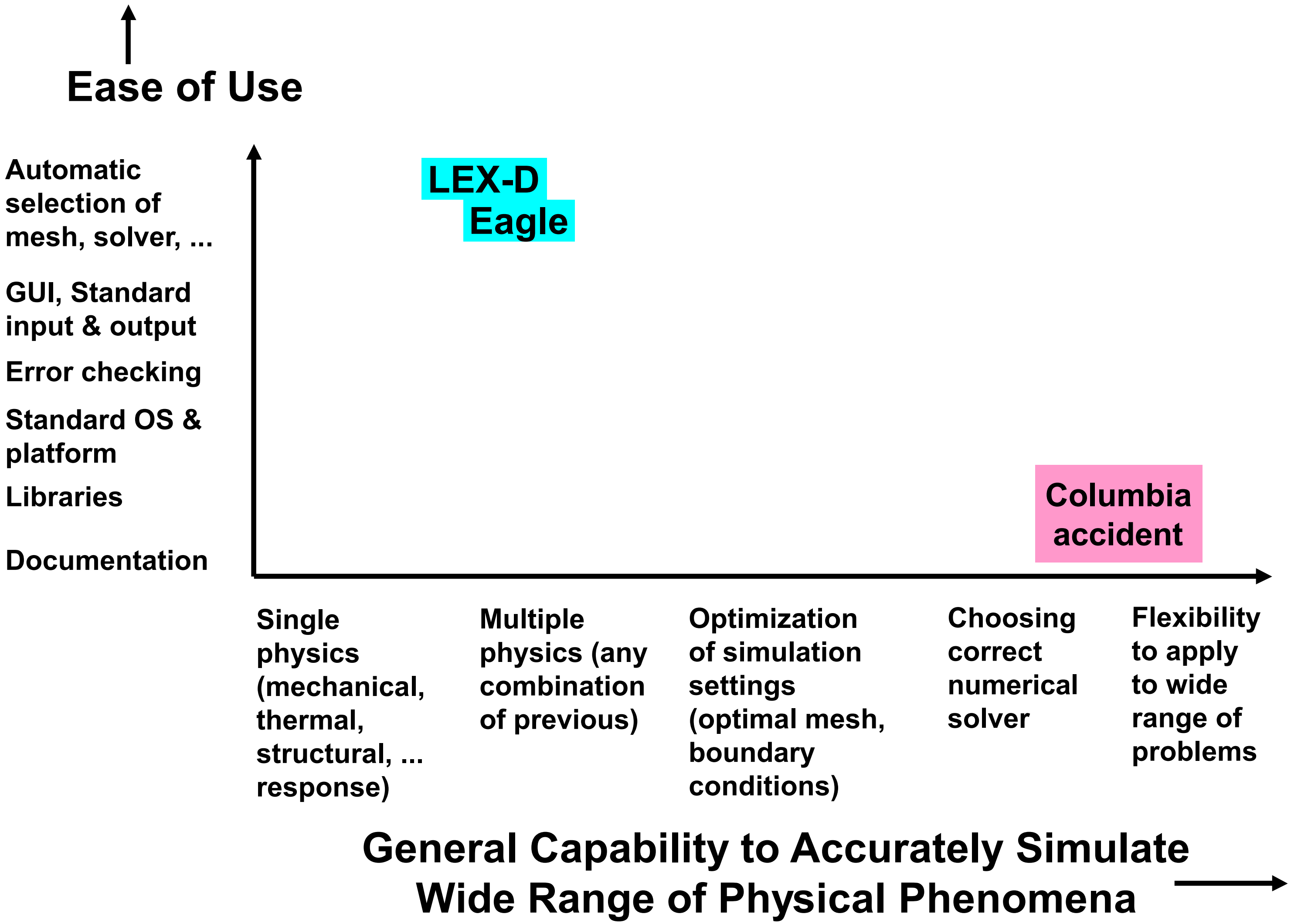
Code Space within Conceptual Framework



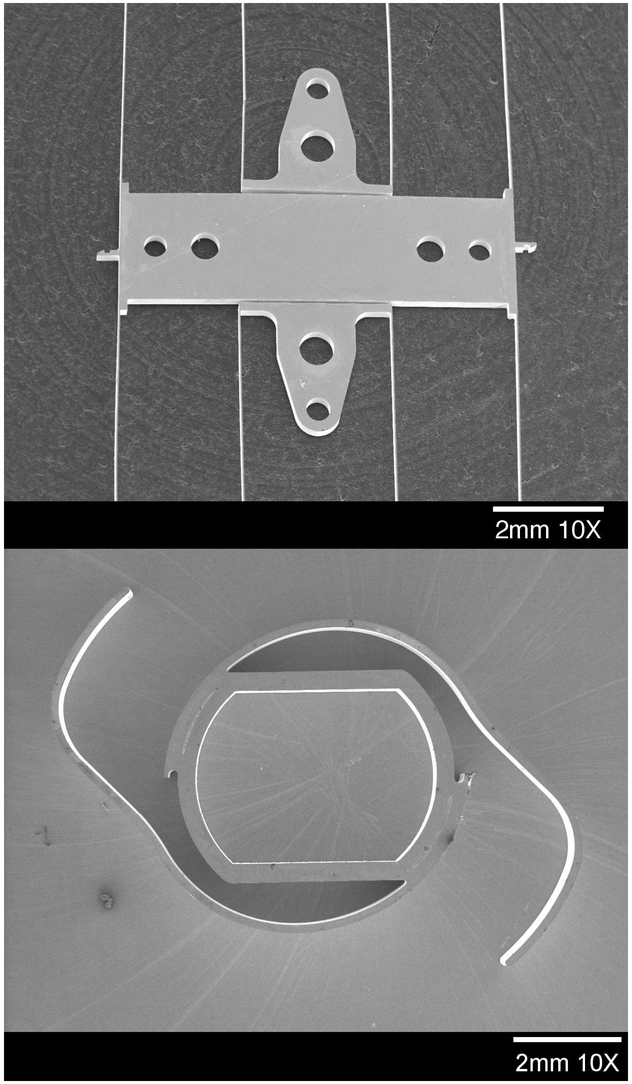
Code Space within Conceptual Framework



Examples of Analysis Codes for Designers and for Computational Analysts



Design Code LEX-D, LIGA EXposure & Development



Micrographs courtesy of Nancy Yang, SNL
Work by Stewart Griffiths, SNL

LIGA parts are formed by electrodepositing in a PMMA mold.

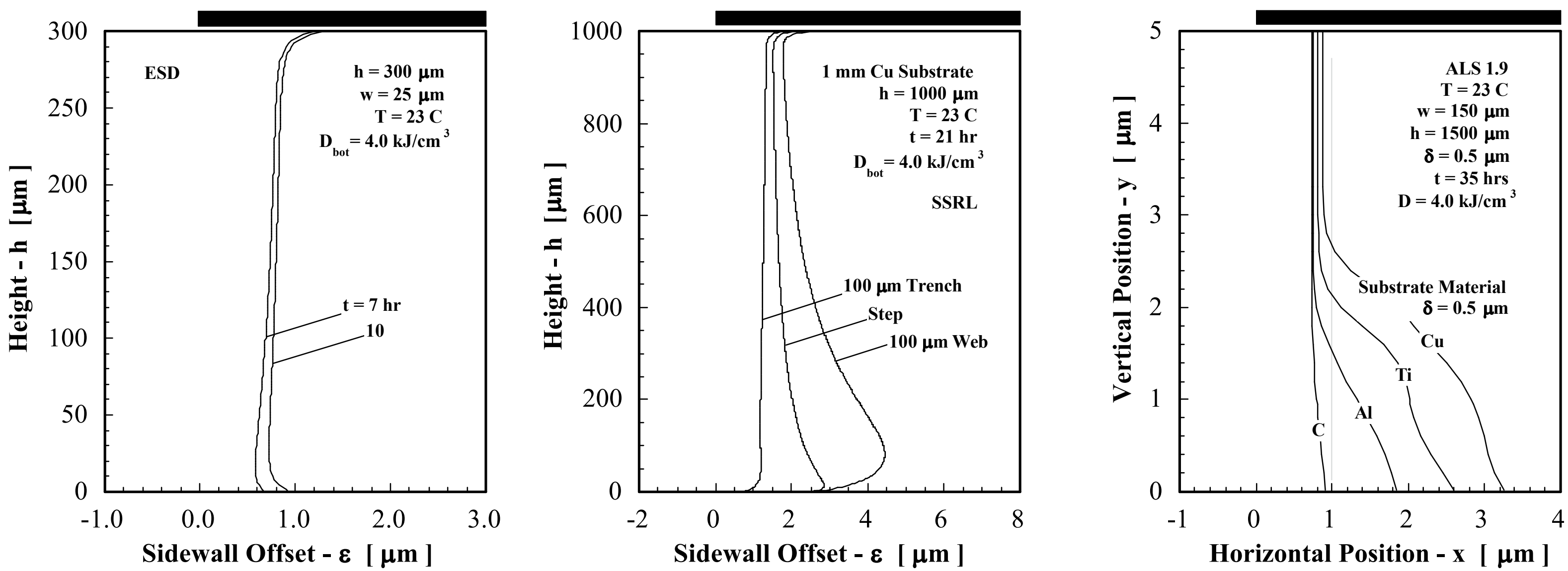
Mold is formed by lithographic techniques
- **Exposing to synchrotron X-ray radiation**
- **Developing to etch away exposed regions**

Synchrotron, exposure and development settings:
dose details, heating, secondary radiation, material properties, synchrotron spectrum, mirrors, absorber thickness & adhesion, substrate properties, … 11 pages of settings

Easy to use: runs on Mac & PC, GUI, general LIGA process knowledge is required.

Design Code

LIGA Mold Design
Sample calculations of final sidewall profile



effect of excess development time -- sidewall photo-e

effect of feature geometry -- substrate fluorescence

effect of substrate material -- substrate photo-electrons

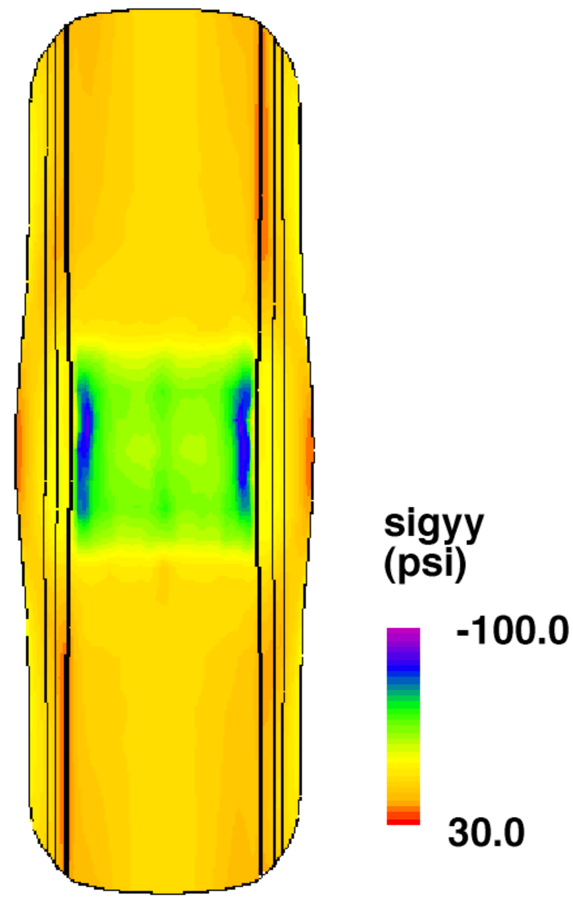
Work by Stewart Griffiths, SNL

Goodyear Design Process Before Partnerships

- **Design Process**
  - Tire Designer Develops Design Concept
  - Prototype Tires Built (3-4 months)
  - Prototype Tires Tested (1 months)
  - Iterate on Design
  - Repeat Process 4-5 times
  - Multiple OEM Submission
- **Computational Simulation**
  - Limited Fidelity Models
  - Many Assumptions that were hard to validate
  - Long Run Times (weeks)
  - Long Model Creation Times (months)
  - Inflate, Deflect

Past: inflate, deflect

70,000 element model



Work courtesy of Martin Heinstein, SNL

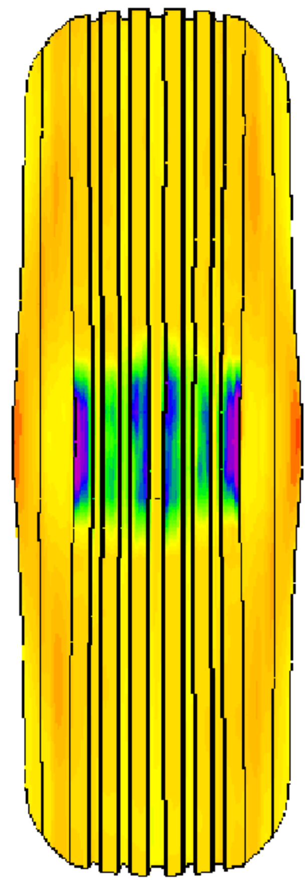
Eagle was developed in partnership with Goodyear

Computational Simulation

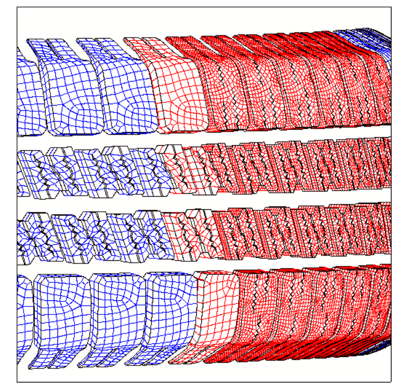
- Increase Model Complexity by Several Orders of Magnitude
- Reduce Model Assumptions Substantially
- Decrease Computational Run Times by 2 Orders of Magnitude (day)
- Automatic Mesh Generation (hour)
- Automatic Coupling between Solid Geometry, Meshing, Mechanics Codes, and Visualization of Results

Present: inflate, deflect, roll deflate, obstacles

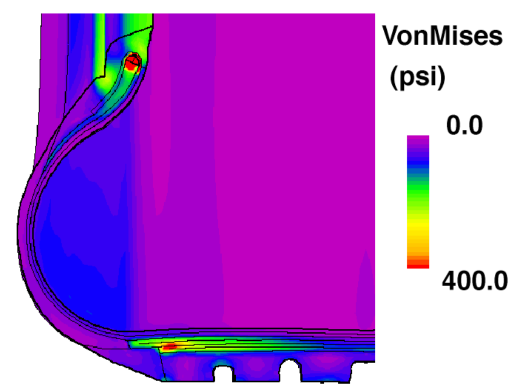
Higher fidelity 280,000 element model



- includes tread



- detailed results…



GOODYEAR

Work courtesy of Martin Heinstein, SNL

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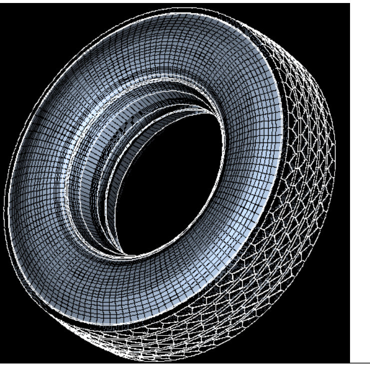
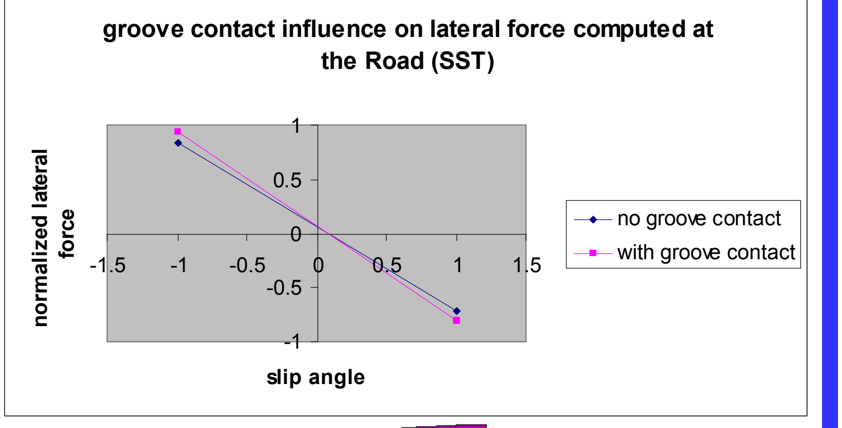
Design Code

Modeling Has Become Essential to New Design Process

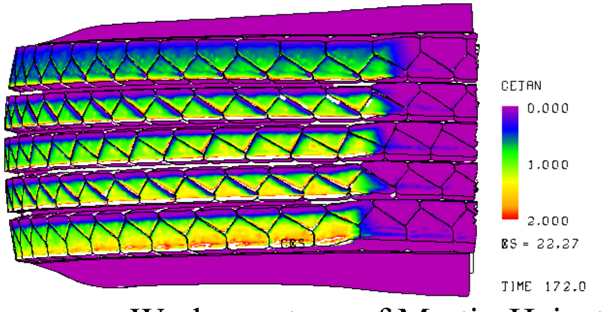
- Tire Designer Develops Design Concept
- Automatically Generated Meshes and Models
- Computational Simulations Used to Evaluate Design Concept
- Re - Design
- Repeat Process





➢ One set of Prototype Tires Built

➢ 1 Successful OEM Submission



Work courtesy of Martin Heinstein, SNL

GOODYEAR

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Application of general codes by experts

Columbia Orbiter Accident Investigation

- Ultimate goal: *to provide"piecewise integration" of key scenario events to determine the plausibility or implausibility of the candidate failure scenarios*
- Three parts to simulation investigation:
  1. Materials response to impact
  2. Areodynamics and heating due to impact damage
  3. Thermal response to heating
- Target of current analysis: Determine aerodynamic and heating behavior of the Shuttle Orbiter during aerobraking maneuvers
- Methodology: Direct Simulation Monte Carlo method
- Results: Flowfield simulations at representative re-entry trajectory points

Work by Michael Gallis, SNL

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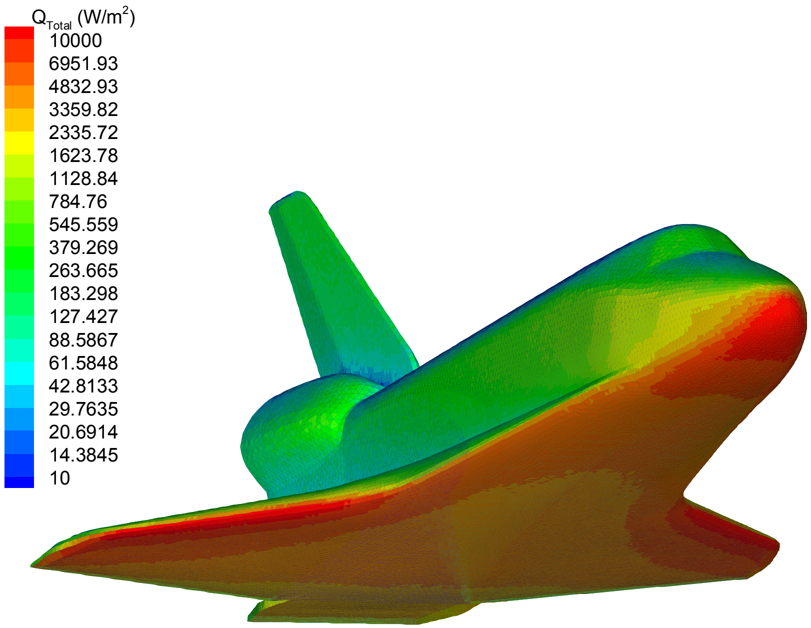
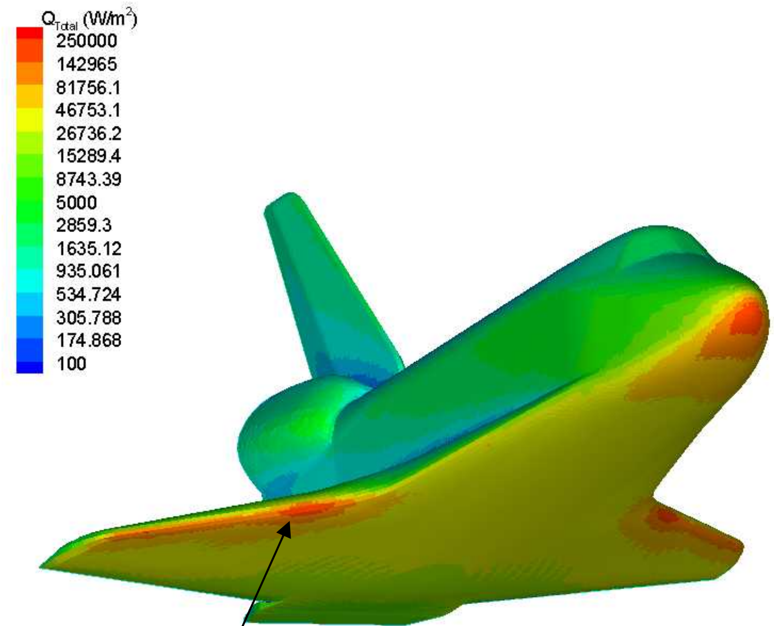
Analysis of flight trajectory

DSMC simulations were performed at two points of the entry trajectory



350 kft flowfield
Surface heating



300 kft flowfield
Surface heating

Two shock waves converge to give highest heating here

Work by Michael Gallis, SNL

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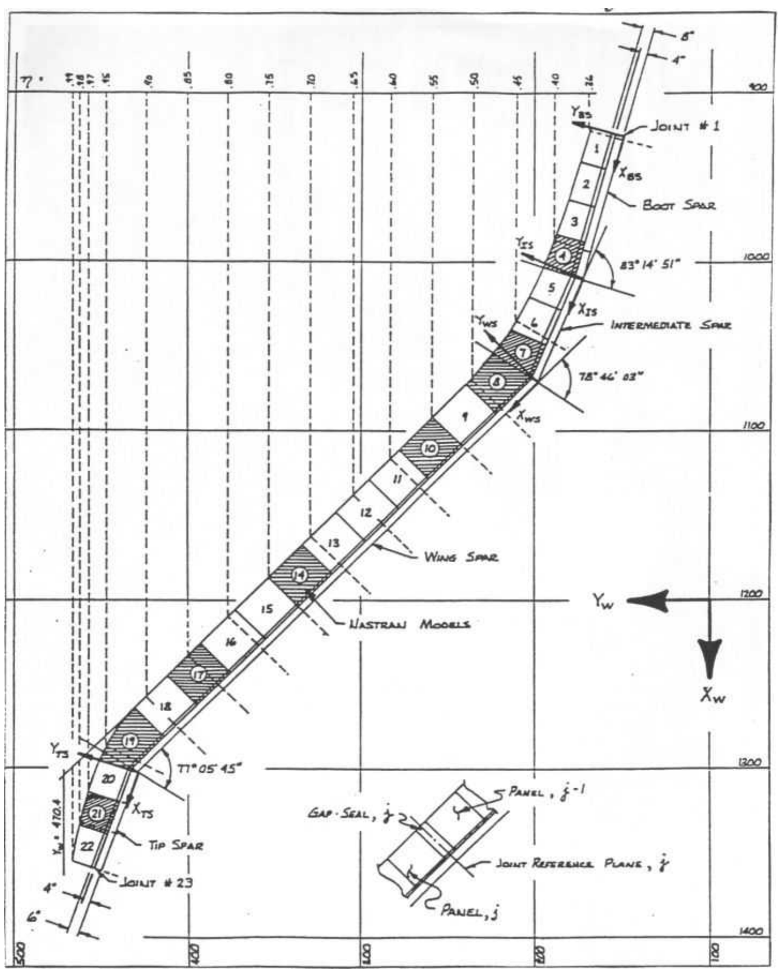
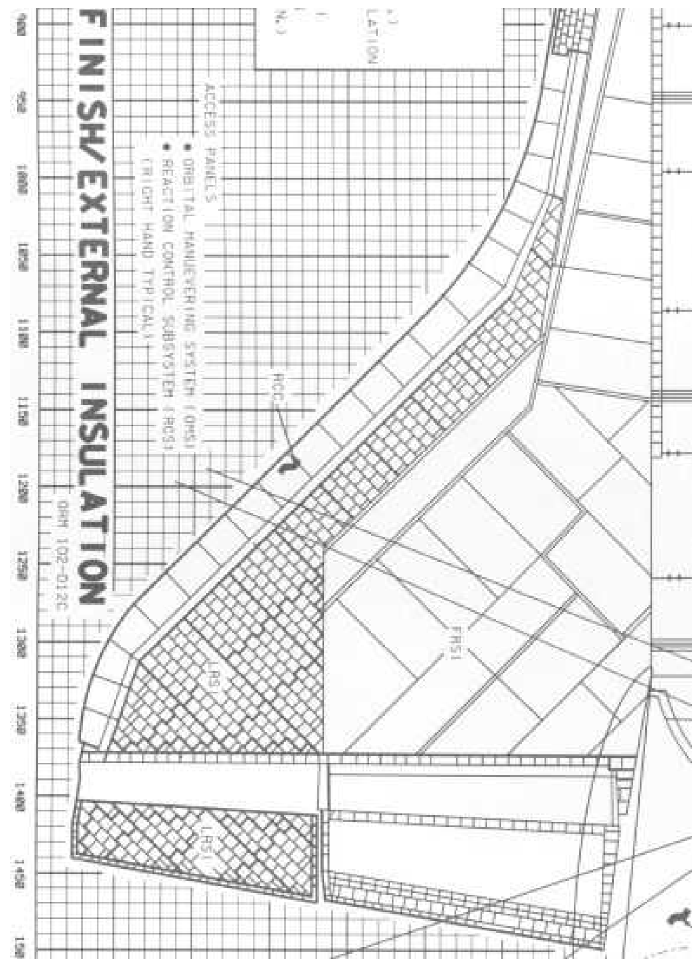
Wing geometry

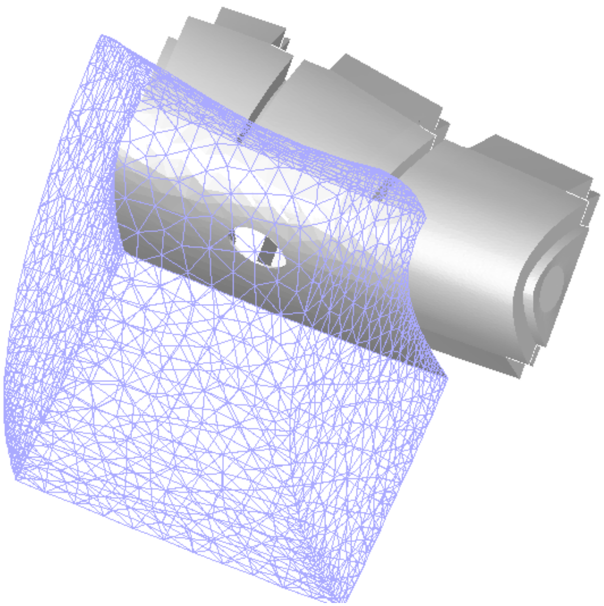




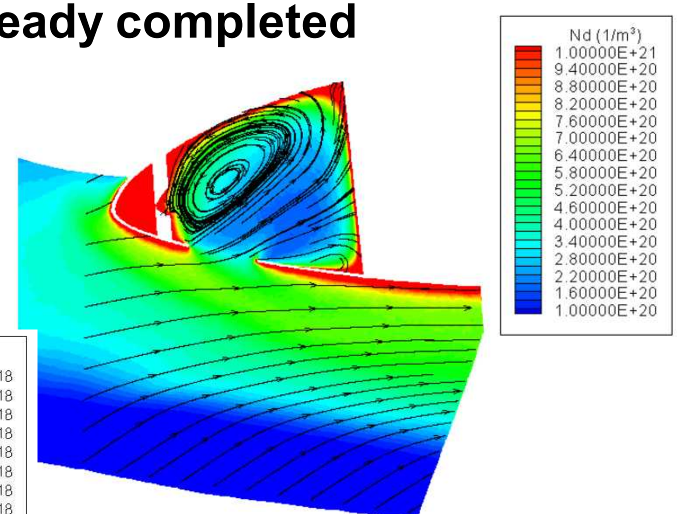
Work by Michael Gallis, SNL

Analysis by expert

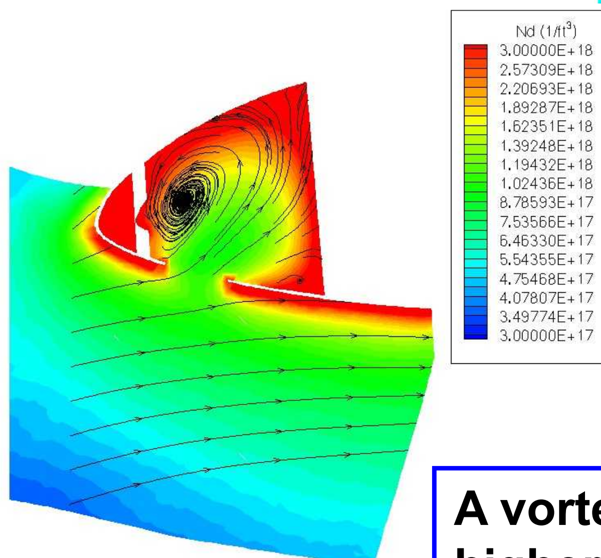
Flow Through a 10-Inch Hole in the Wing Leading Edge



External inflow boundary conditions extracted from 350 kft and 300 kft full-length shuttle cases already completed



300 kft



350 kft

A vortex in the hole lead to much higher damage than anticipated

Work by Michael Gallis, SNL

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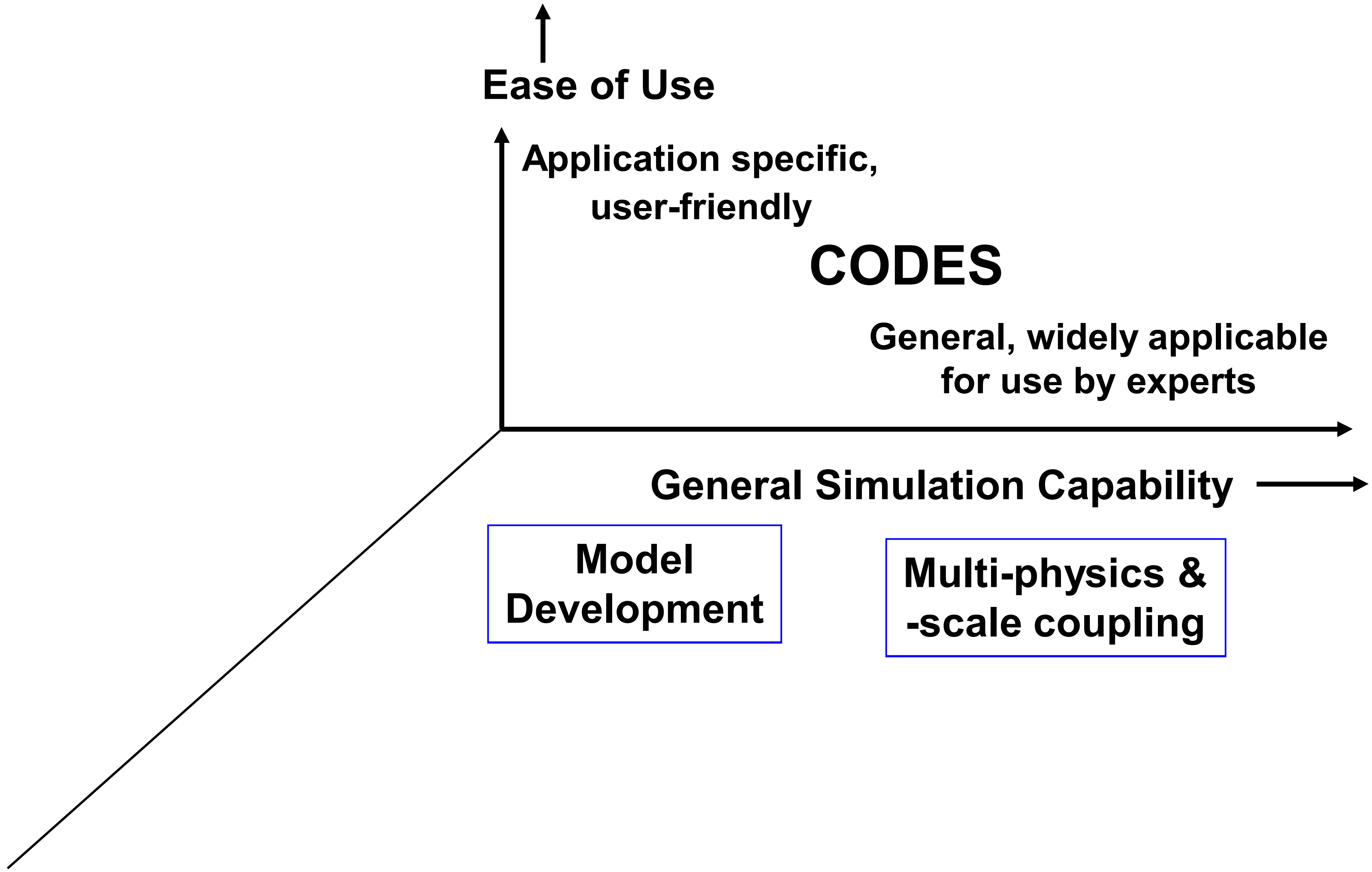
What does it take to build codes?



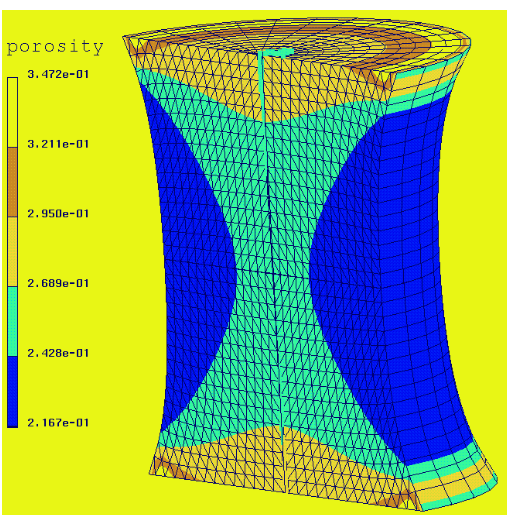
Model Development

Many powder processing techniques lead to anisotropic sintering

Powder processing that can result in anisotropic sintering:

- **Uni-directional pressing**
- **Tape casting**
- **Injection molding**

However, most sintering simulation use constitutive equations that treat it as an isotropic problem with P_L and ζ as scalar quantities.



$$\frac{dV}{V_o dt} = \frac{-P_L}{\zeta}$$

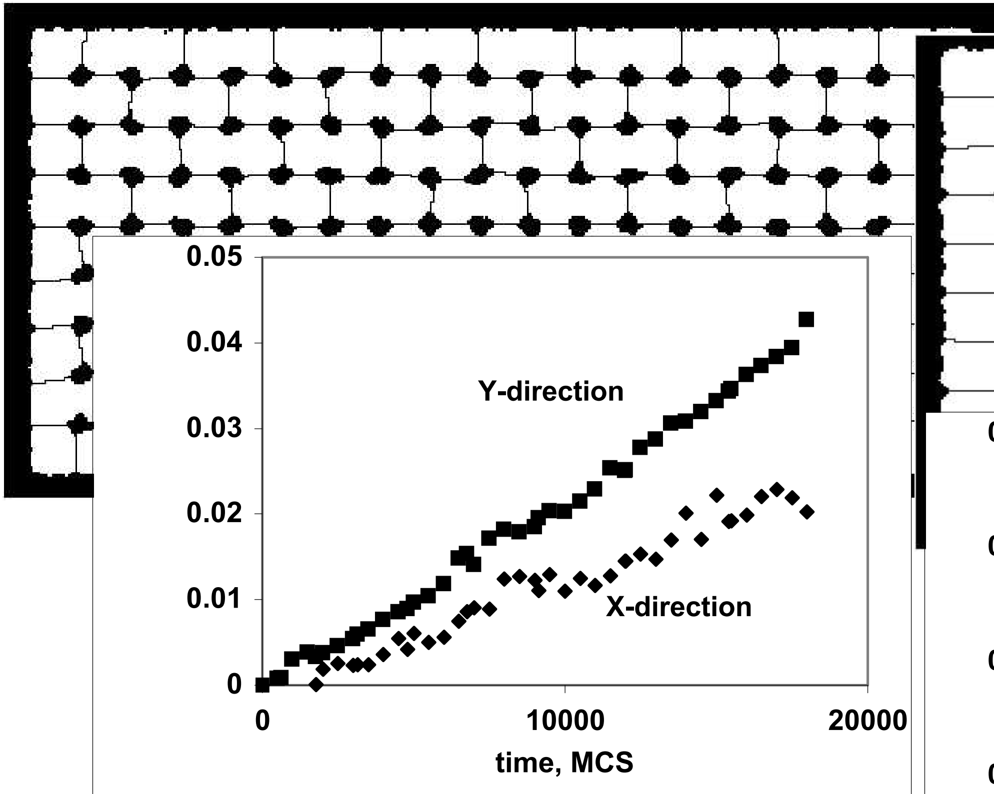
sintering stress

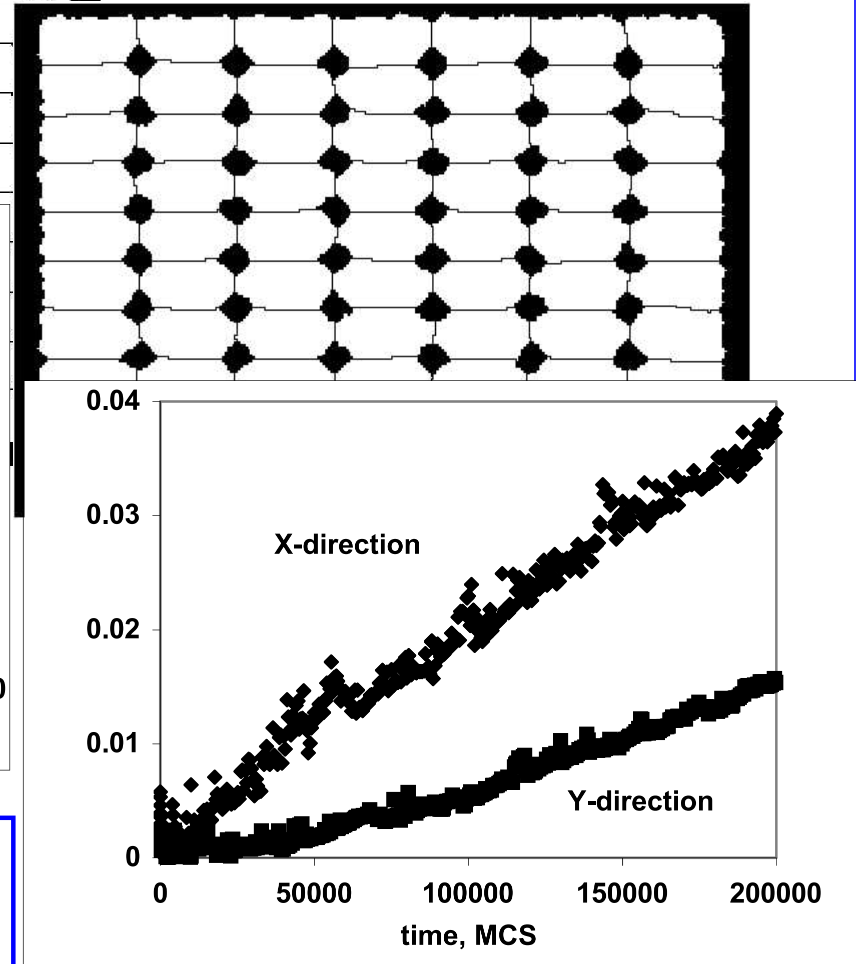
Shrinkage rate

bulk modulus

Model Development

Very similar microstructure can give exactly opposite shrinkage behavior

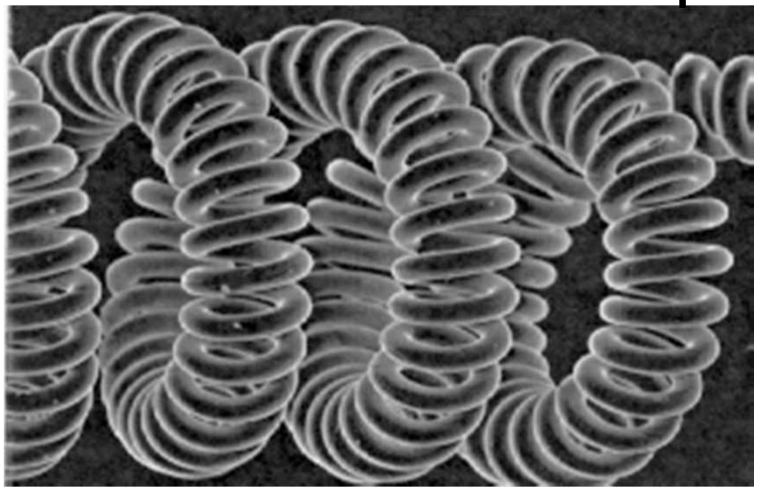




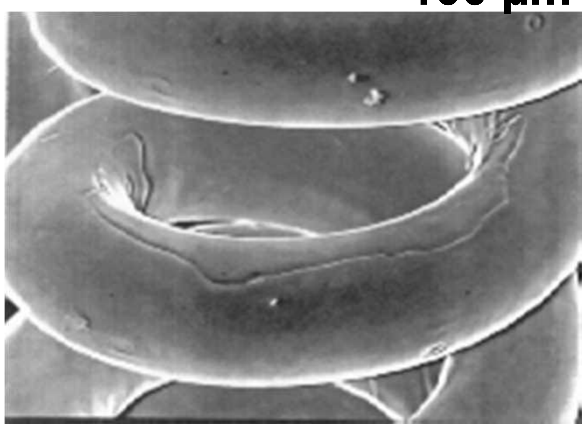
[P_L] and [ζ] are correctly treated as tensor quantities. We are developing techniques to do so.

Recrystallization controls the properties of tungsten lamp filaments.

500 μm



100 μm



- Lamp filaments are a coiled coil of 55 μm diameter tungsten wire
- 40% plastic strain imparted in final coiling
- Filaments operate at 0.8 T_m under shear stresses up to 25 MPa

⇒ Recrystallization occurs during first lamp power up

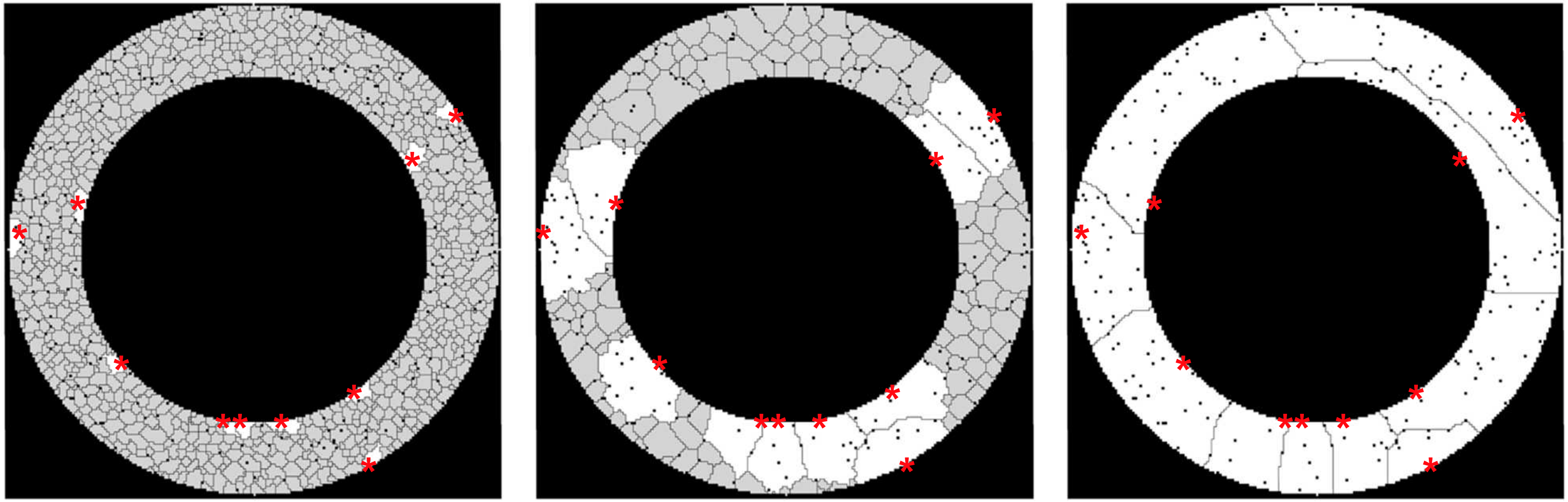
- To minimize creep in service, tortuous boundaries, radial to the filament axis are desired

Micrographs courtesy of John Selverian, Osram-Sylvania
Work of Elizabeth Holm, SNL

Model Development

Recrystallization in lamp filaments depends on nucleation parameters

Example: 2-D toroidal specimen, recrystallized nuclei at surface, uniform strain with unrecrystallized H/g=1, 0.5 v/o K bubbles



t=1000 timesteps　　t=10,000　　t=100,000

Recrystallized structure is relatively insensitive to strain energy distribution, pinning particles, prior grain structure, etc.

Nucleus position, frequency, and growth behavior govern final grain boundary positions.

Work of Elizabeth Holm, SNL

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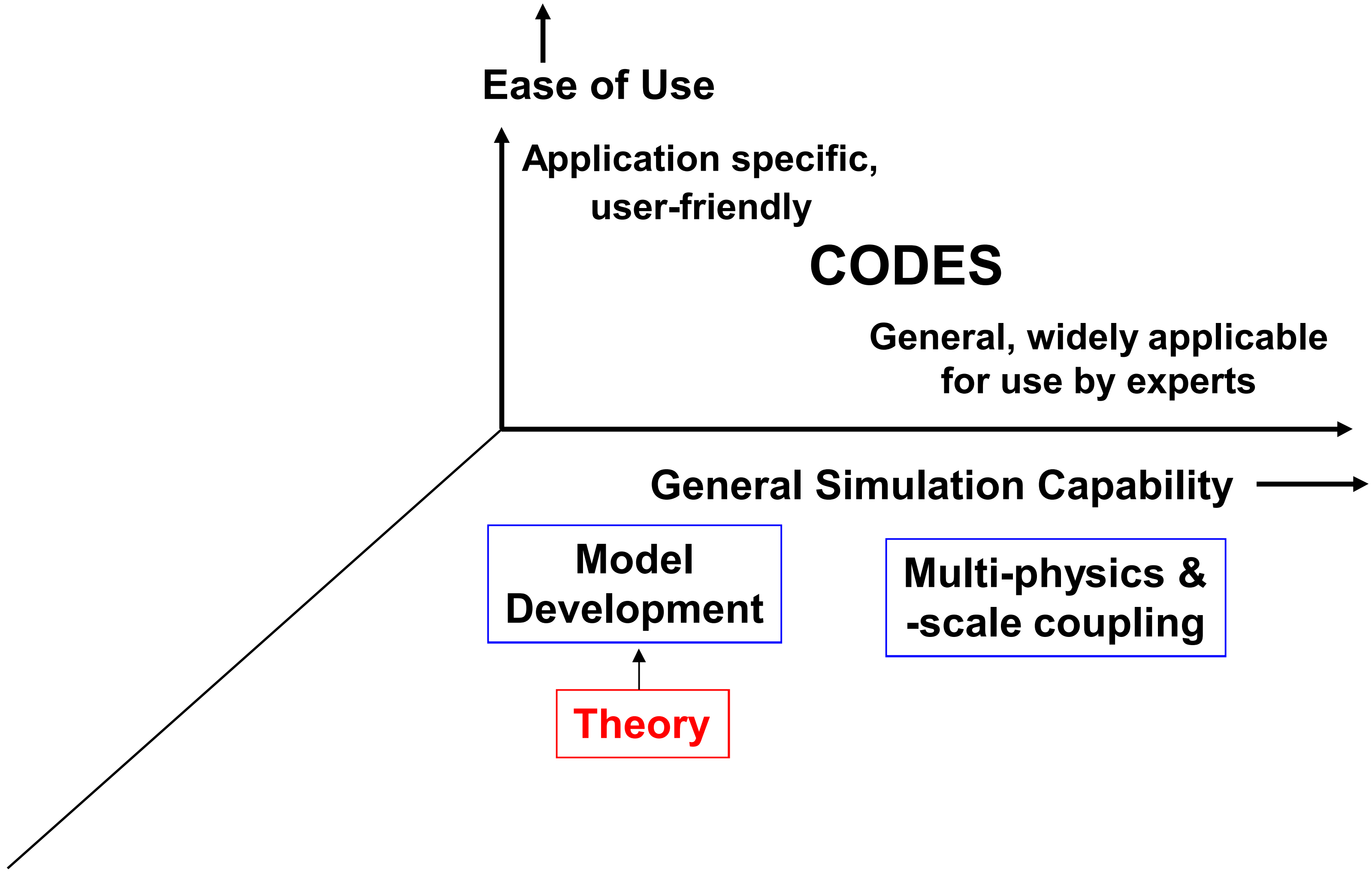
What does it take to build codes?



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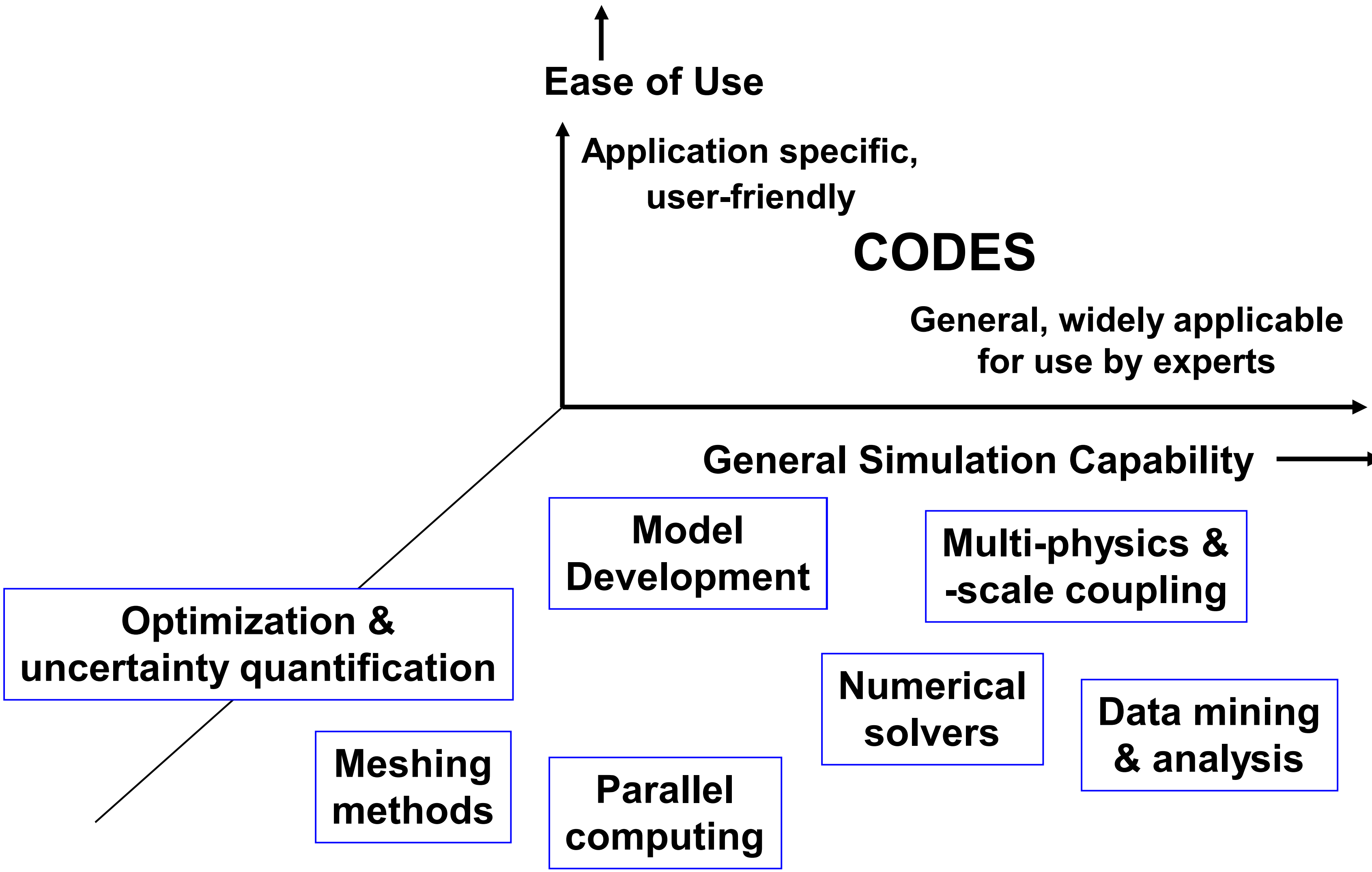

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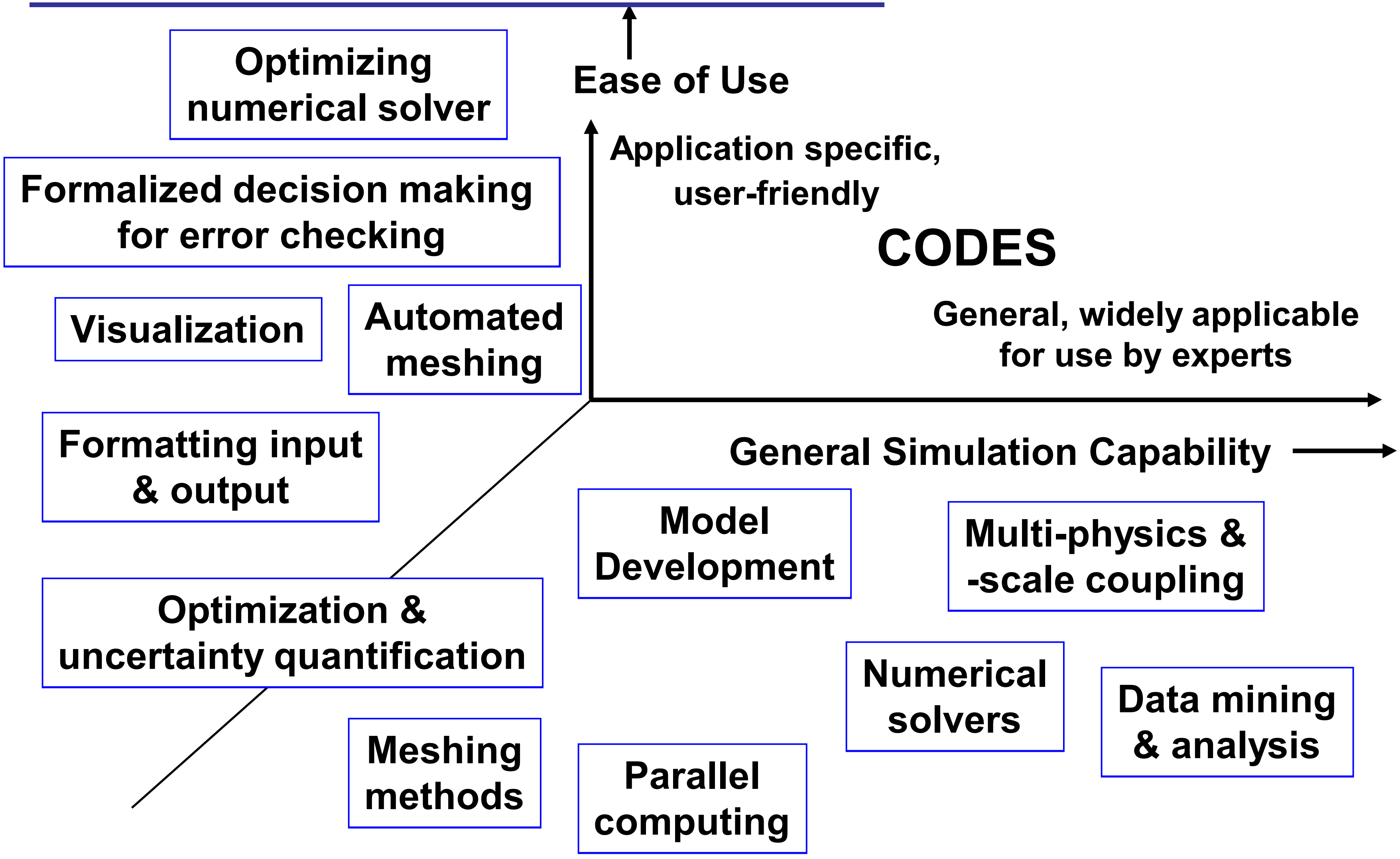
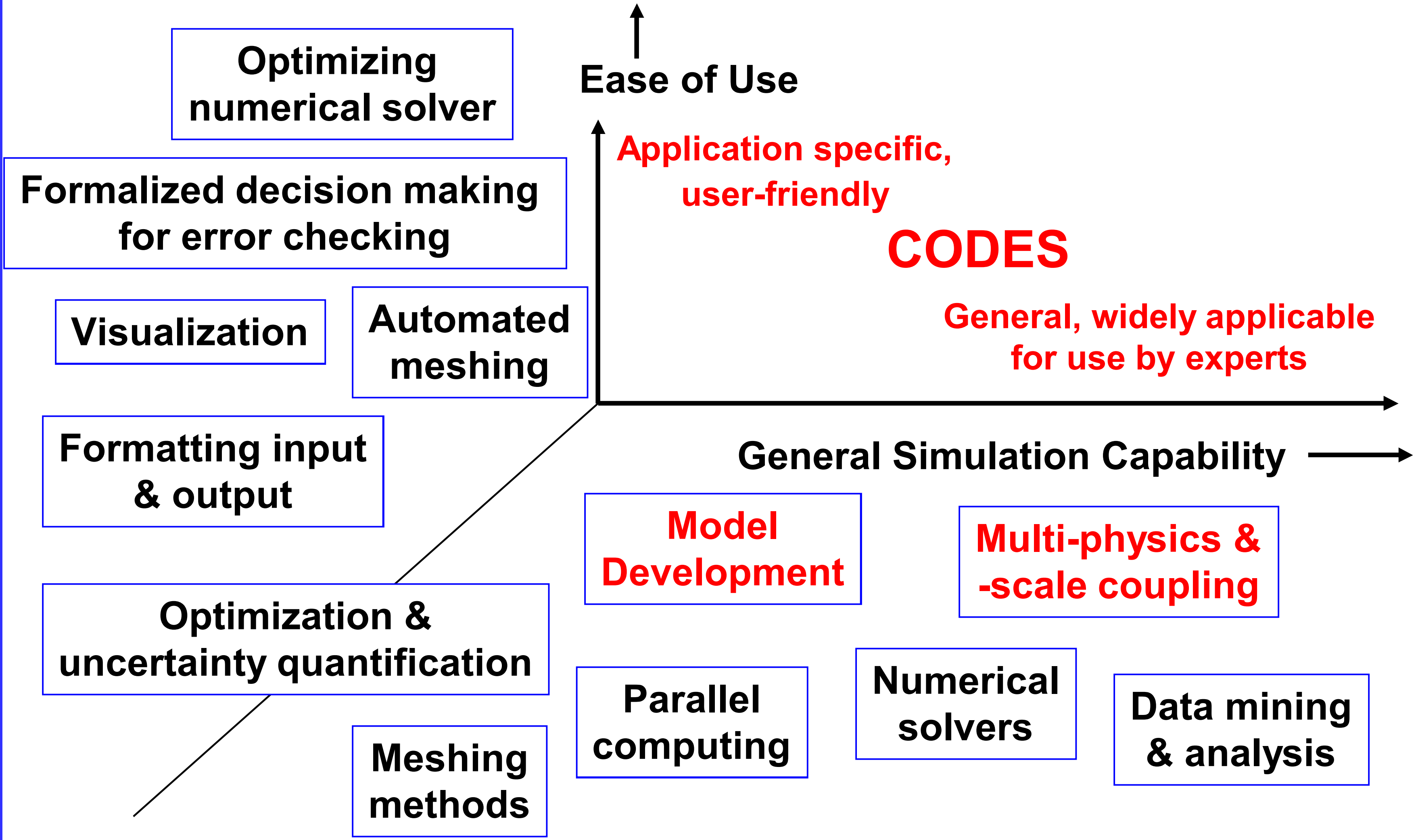
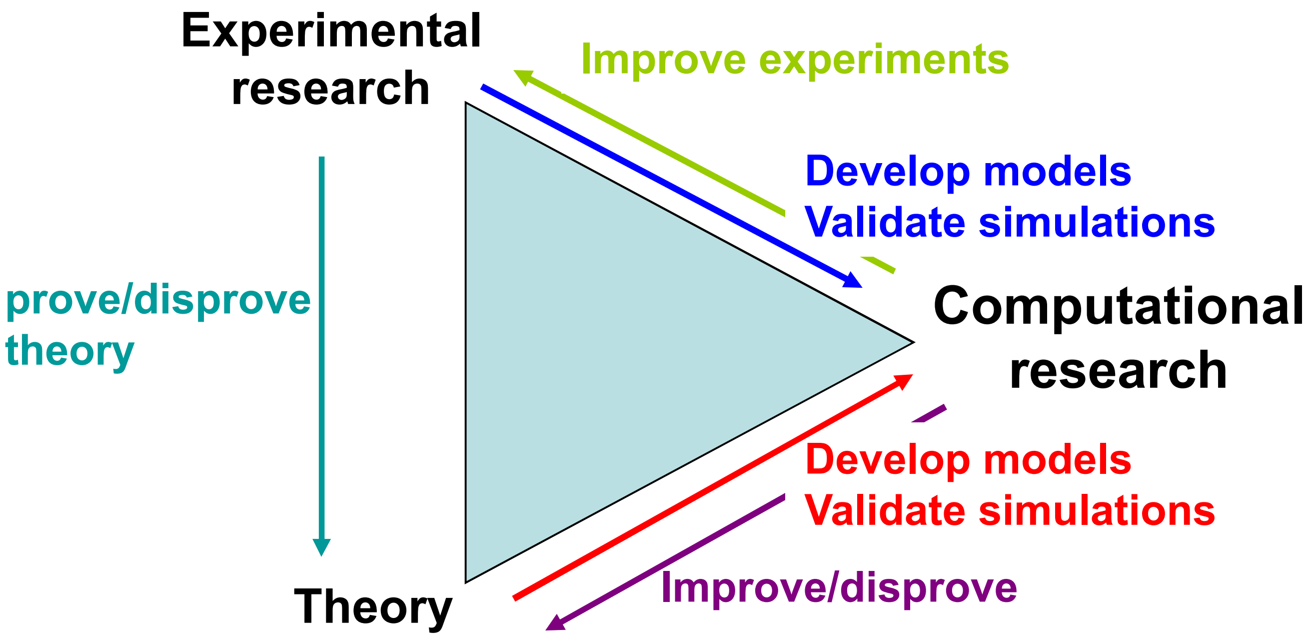


Models and codes must be based on and verified by experiments and theory



Conclusions

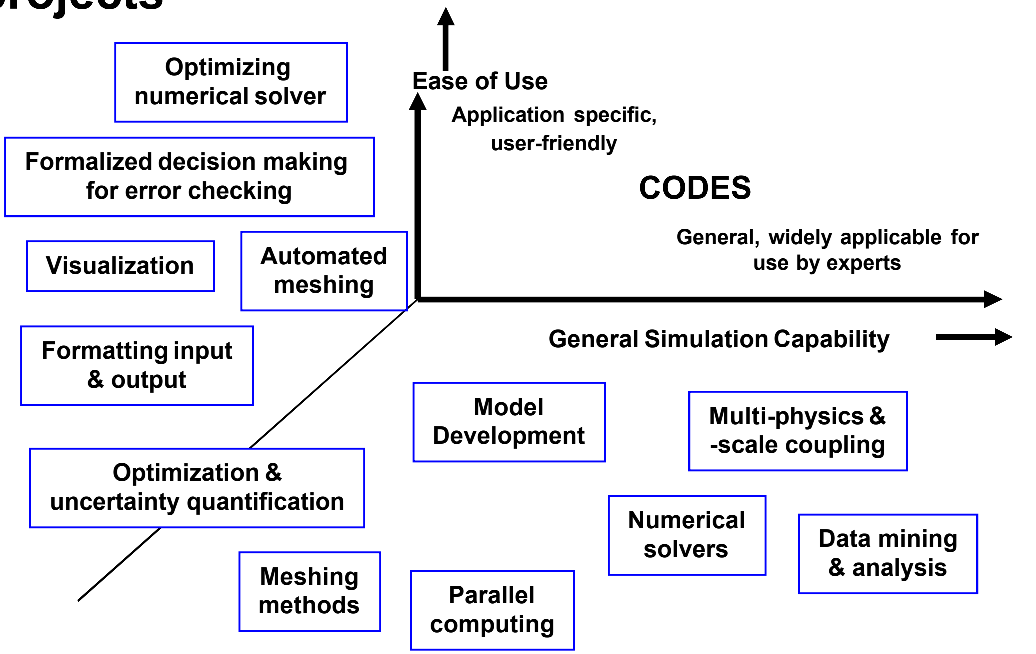
Any good comprehensive research and development effort must integrate experimental, theoretical and computational work



This framework describing experiment-theory-computation relationship is widely accepted in the scientific and engineering communities

Conclusions (Cont'd)

However, we do need better frameworks to facilitate decision making for specific programs and projects



Example: Integrating simulations will cost less!

Model development, numerical solvers, meshs/digitization, visualization, scaling by parallelization, uncertainty quantification, …. are costly

Modeling and Simulations allow one to gain understanding and/or improve designs that would otherwise be virtually impossible