

# Contact Mechanics for Integrated Circuit Manufacturing

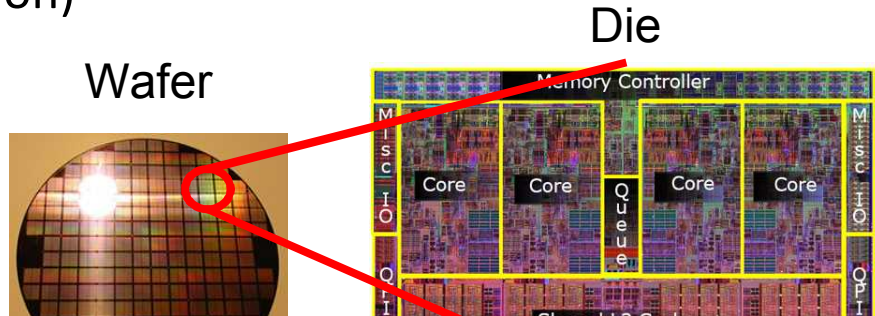
Jonatan A. Sierra Suarez PhD

# Outline

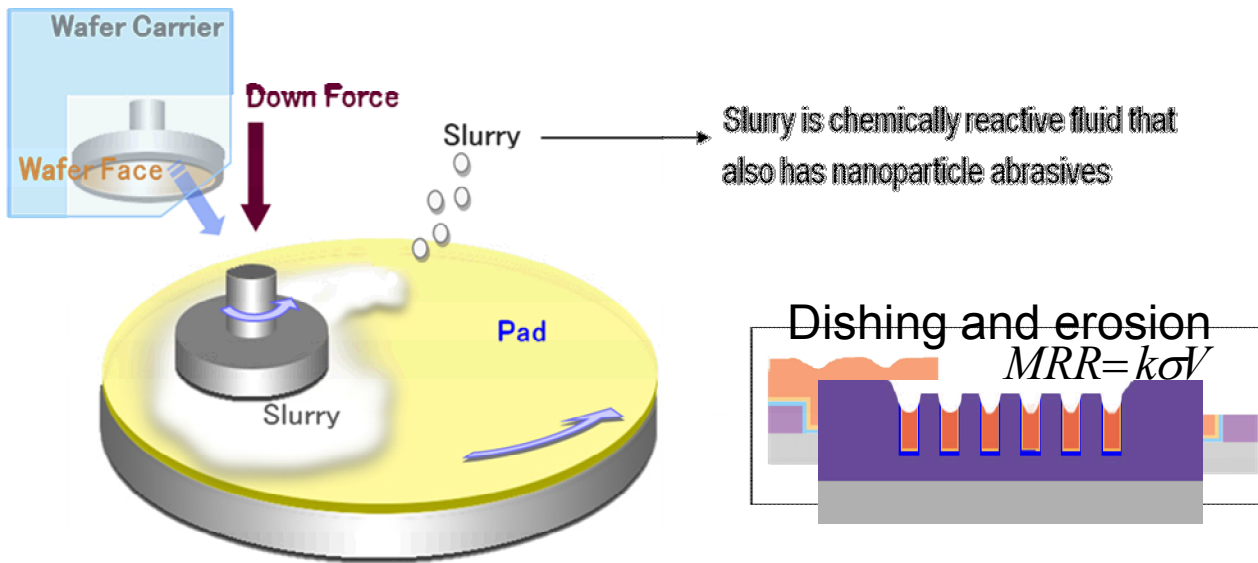
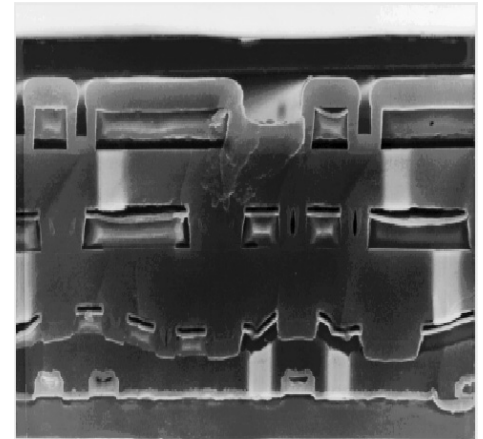
- Introduction to IC Manufacturing
- High Fidelity Contact Mechanics: General rough surface contact applied to CMP
- Contact Mechanics at the MESAfab

# Chemical Mechanical Polishing (CMP): Basics

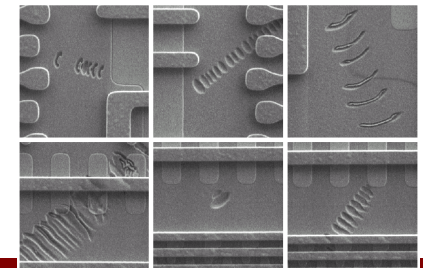
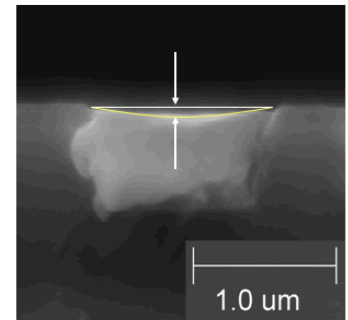
- CMP is used extensively to achieve planarity
- Leads to yield losses through systematic (dishing and erosion) and random defects (micro-scratches, particle contamination)



Defect SEM Images\*



Courtesy  
3M, Hitachi,  
TD- Perl



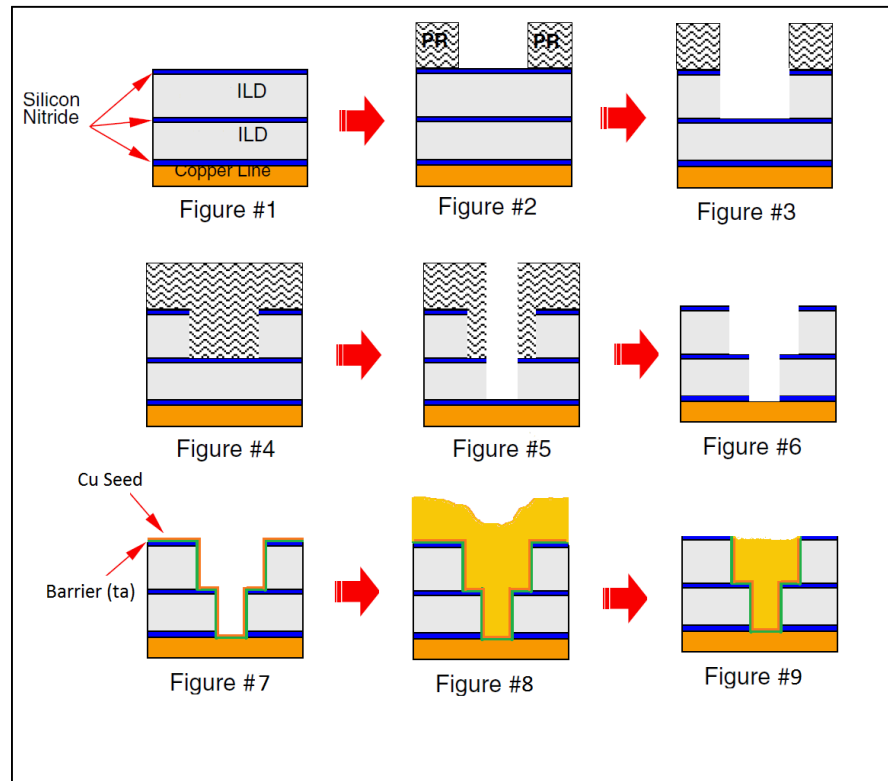


# Background: Manufacturing Processing Flow

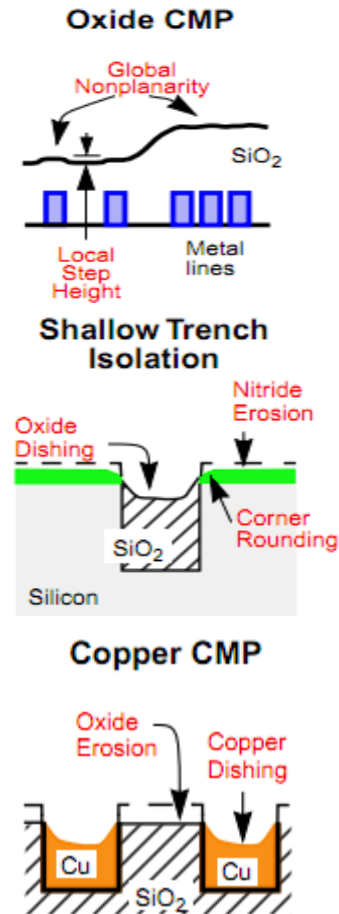
All unit processes below will be performed multiple times during the fabrication of IC devices

- CMP
- Deposition
- Etching
- Photolithography

## Dual Damascene Process Steps (BEOL)

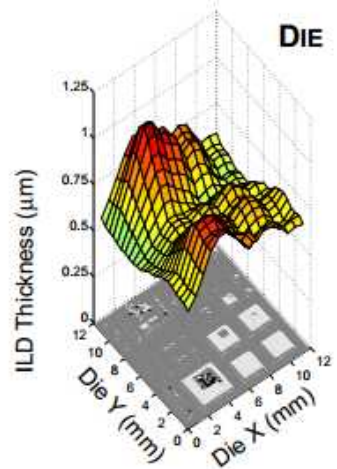
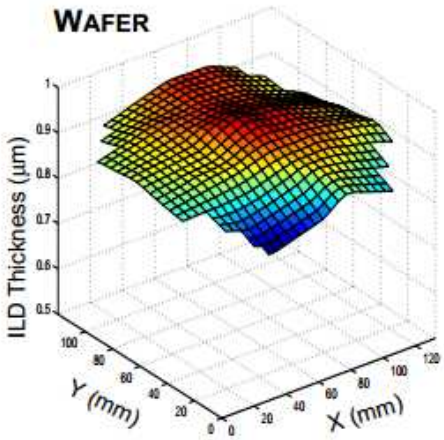


## CMP Uses



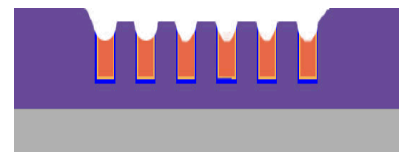
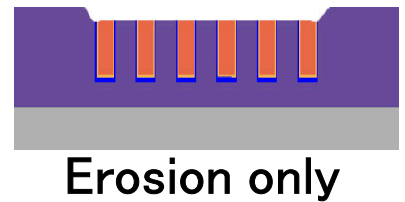
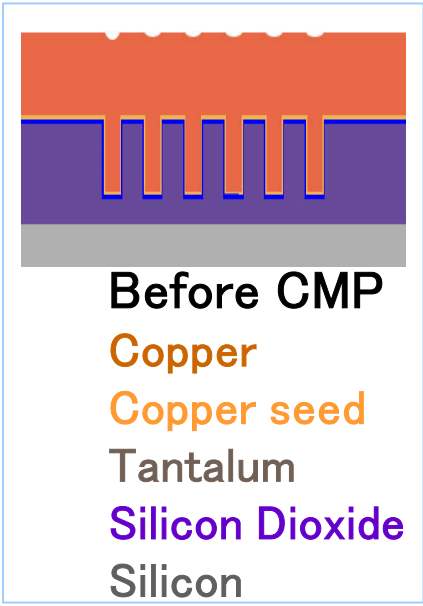
# CMP : Non-Uniform Material Removal Rate (MRR)

## Wafer and die non-uniformity



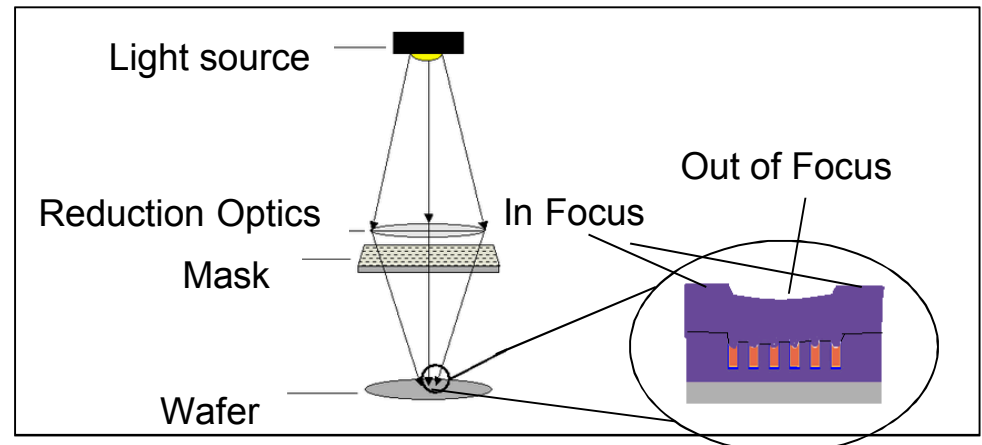
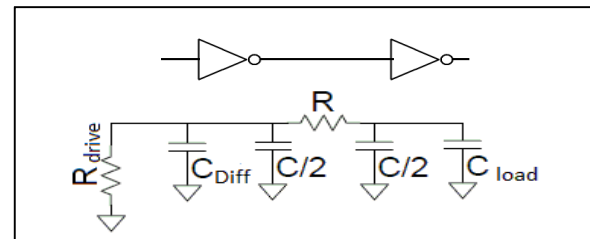
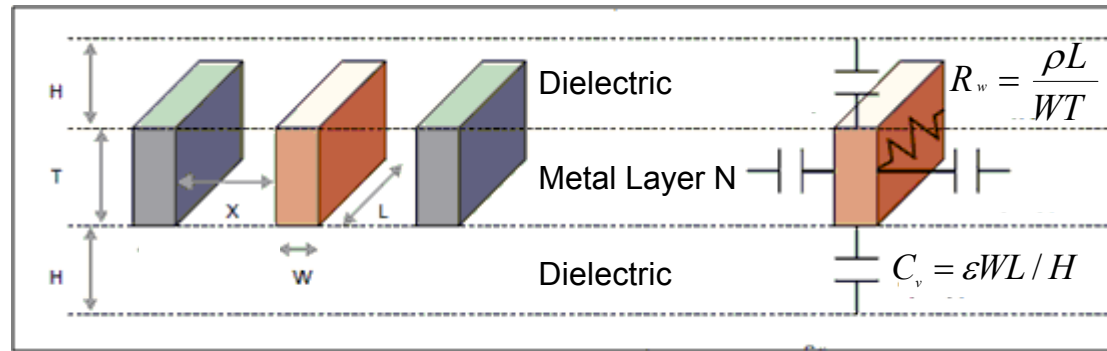
Non-uniformity across scales from Ouma et. al 2002

## Feature non-uniformity



# CMP: Manufacturing Impact

- Dummy fill, dishing, and erosion will raise resistance and capacitance
  - This affects timing and power
- Successful photolithography depends on low topography variation due to depth of focus (DOF)



# Elastic Halfspace Contact Solution for CMP

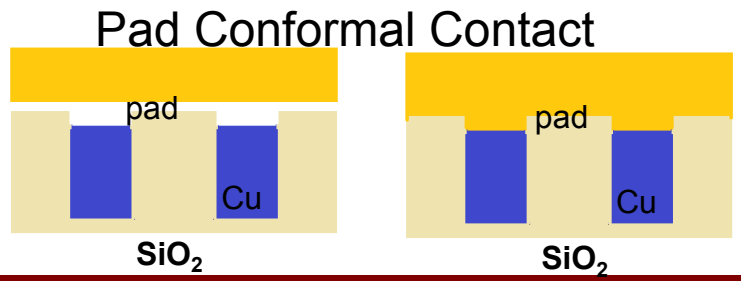
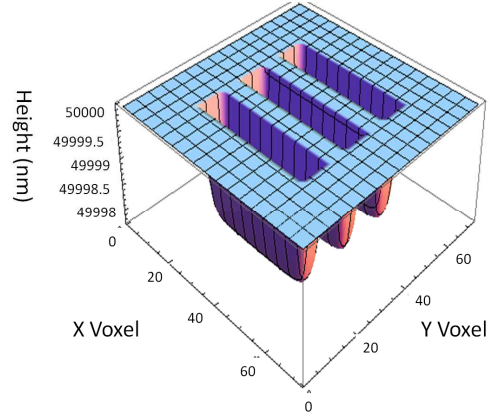
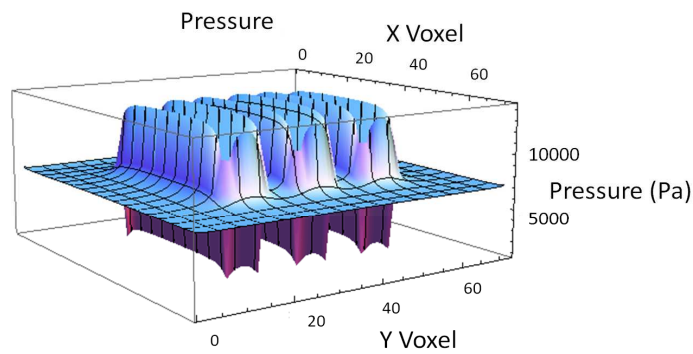
Deflection  $u_z$  at a point in an elastic halfspace due to applied pressure (Johnson 1985):

$$u_z(x, y) = \frac{1 - \nu^2}{\pi E} \iint \frac{\sigma(x', y')}{\sqrt{(x - x')^2 + (y - y')^2}} dx' dy'$$

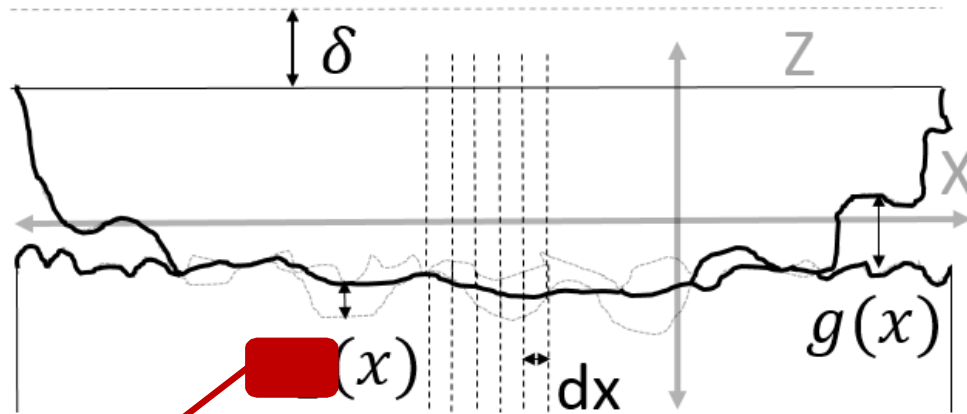
Couple with Preston's wear equation to calculate material removal rate (MRR)

$$MRR = k \sigma V$$

Nomenclature			
<b>u</b>	Surface Deflection	<b>σ</b>	Contact stress
<b>ν</b>	Poisson ratio	<b>k</b>	Preston coefficient
<b>E</b>	Young's Modulus	<b>V</b>	Relative velocity



# Contact Mechanics Formulation



The composite vertical surface displacement:

$$u_z(x, y) = \frac{1 - \nu^2}{\pi E} \iint \frac{\sigma(x', y')}{\sqrt{(x - x')^2 + (y - y')^2}} dx' dy'$$

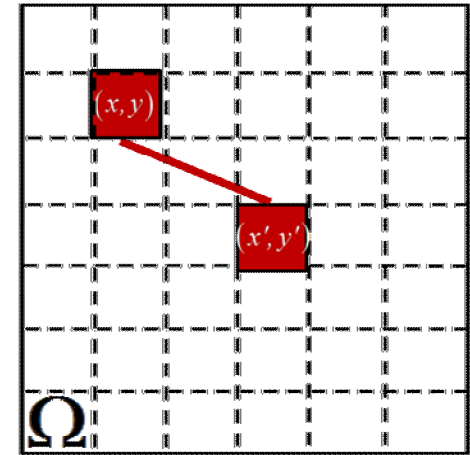
Every element has an influence on all other elements (Johnson, 1985)

Direct matrix multiplication  $O[(N_x \times N_y)^2]$

$$\mathbf{u}_z = \mathbf{C}\boldsymbol{\sigma}$$

Or leverage Fourier analysis  $O[(2N_x \times 2N_y)]$

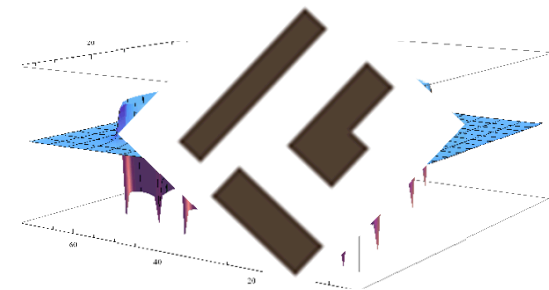
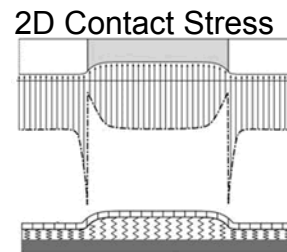
\*Discretized computational domain (view from top)



\* $N_x \times N_y$  elements

\*Graphic: Zenyuk, Kumbur, Litster (2013)

3D Sample Layout

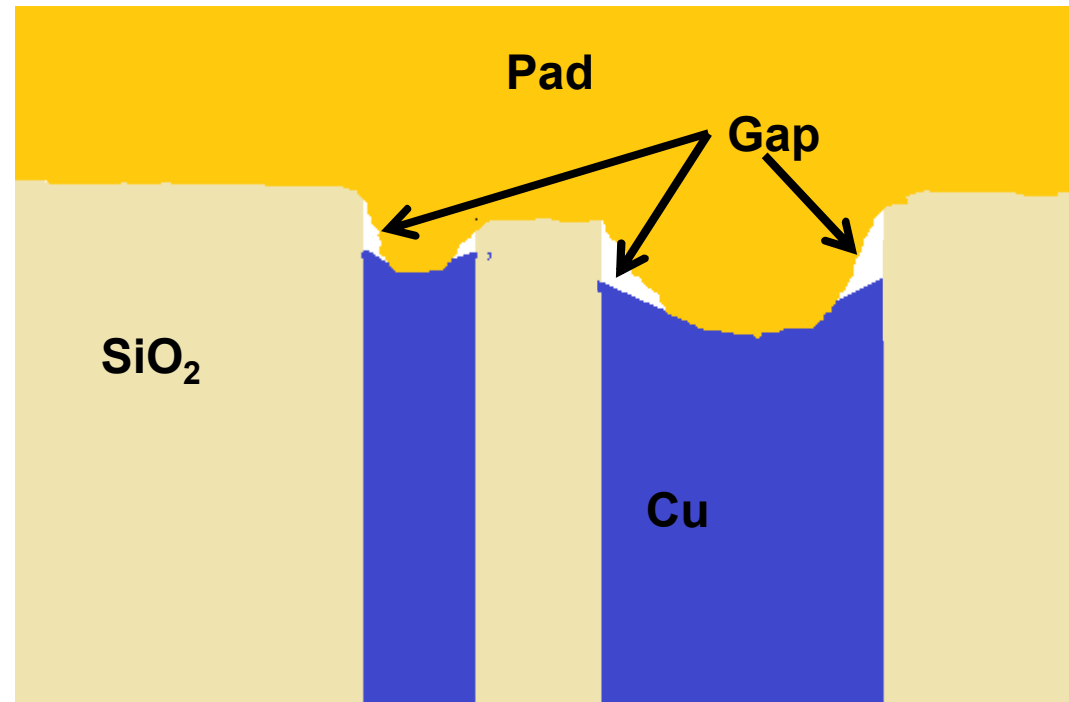


## Fidelity CMP

- Introduction to IC Manufacturing
- High Fidelity Contact Mechanics: General rough surface contact applied to CMP
- Contact Mechanics at the MESAfab

# Conformal Assumption Removal: Two-Body Contact

- Contact is not necessarily conformal
- Remove conformal assumption by treating contact as a general two body problem.



# Deterministic Two-Body Contact

- Two body contact is a linear complimentary problem
  - Multiple methods to solve (Alwood 2005)

$$\mathbf{g} = \mathbf{g}_0 - \delta + \mathbf{u}$$

$$\mathbf{u} = \mathbf{C}\boldsymbol{\sigma}$$

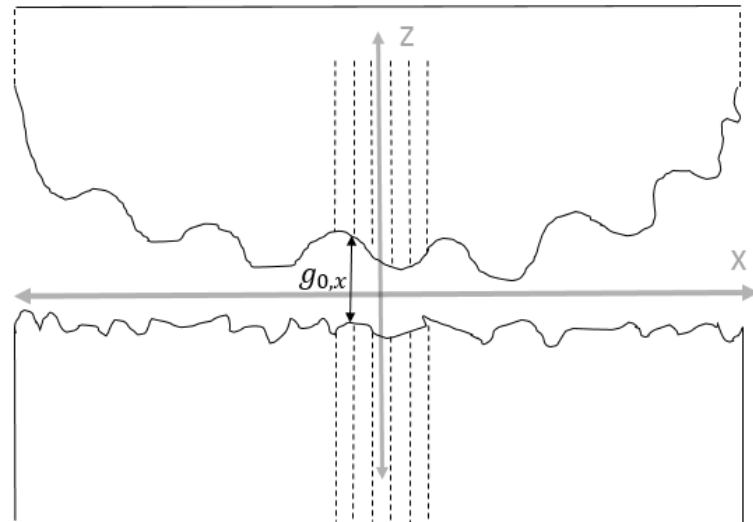
$$\mathbf{g} = \bar{\mathbf{g}} + \mathbf{C}\boldsymbol{\sigma}, \quad s.t.$$

$$\sigma_{x,y} = 0, \quad g_{x,y} \geq 0$$

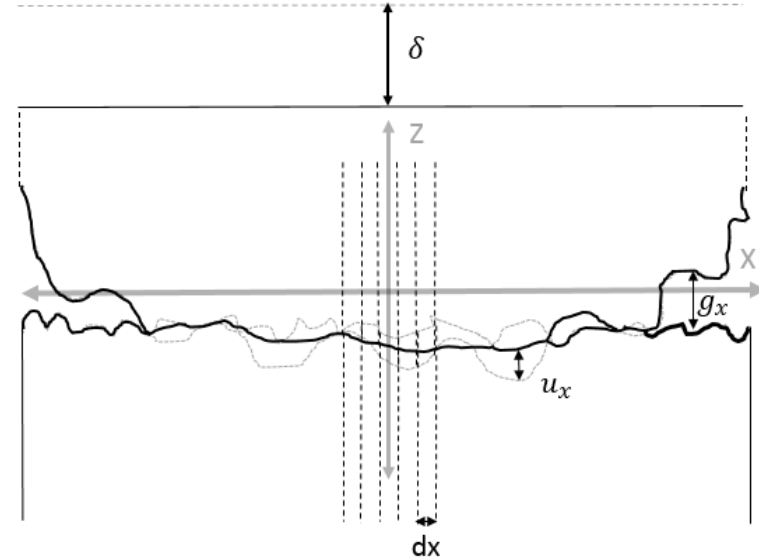
$$\sigma_{x,y} > 0, \quad g_{x,y} = 0$$

$$\Rightarrow \boldsymbol{\sigma} \bullet \mathbf{g} = 0$$

Initial Surfaces

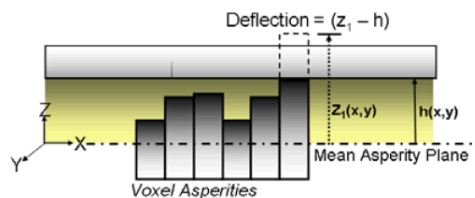


Deformed Surfaces



# Contact Model Comparison

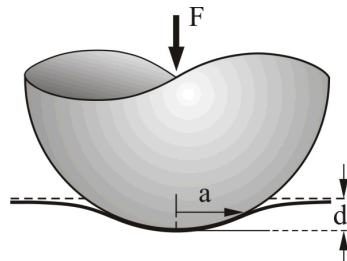
## Winkler



Elastic body is treated as set of linearly independent springs

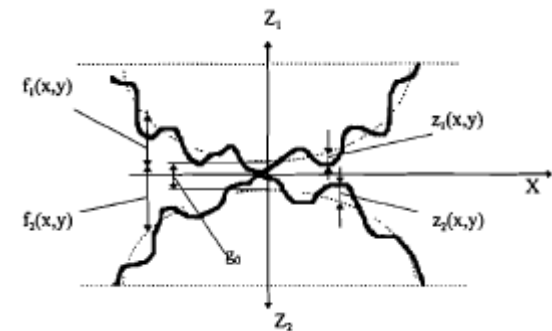
In collaboration with TPES (Prof. Shawn Litster & Prof. Iryna Zenyuk)

## Hertzian



Analytical model to conformal contact geometries such as sphere on sphere contact

## Elastic halfspace with FFT, and constrained CGM (Hu et. al 1999)

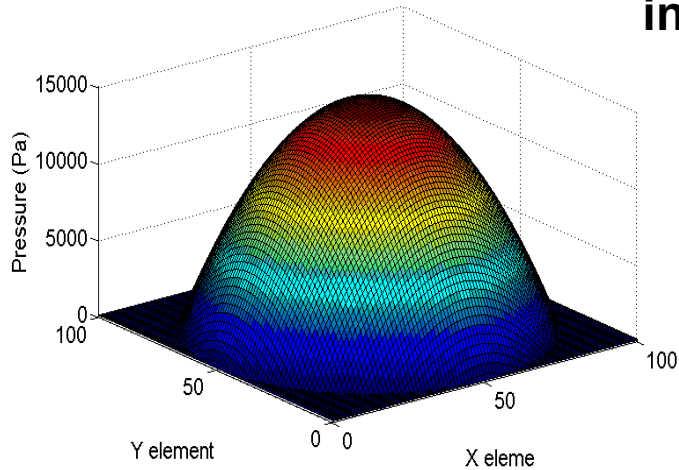


Solves general two body contact by treating the problem as an optimization problem

The CGM fits nicely with computationally efficient FFT

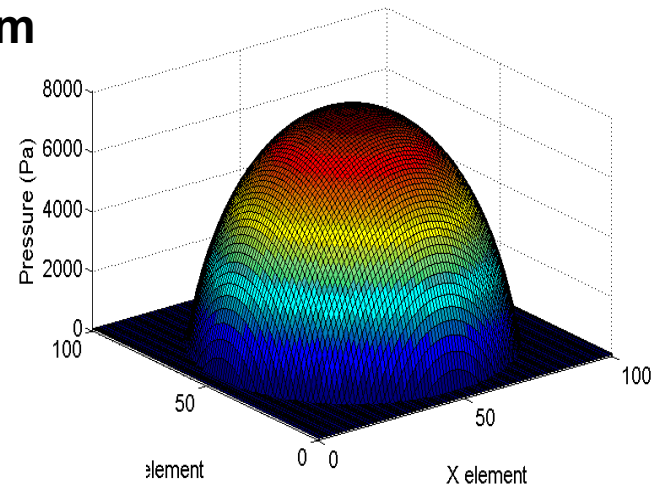
# Error Analysis Between Three Contact Models

## Winkler

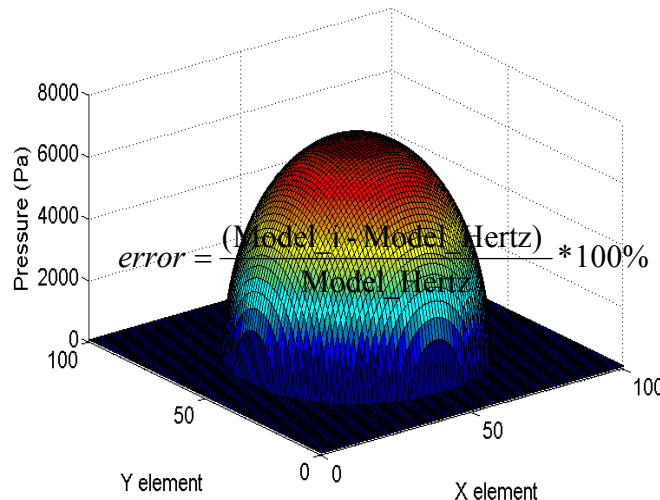


## Pin-On-Disk indentation of 0.5um

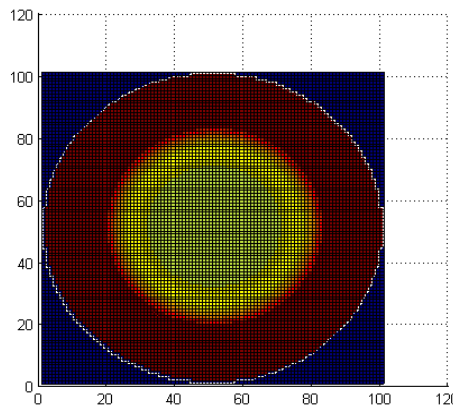
## Hu



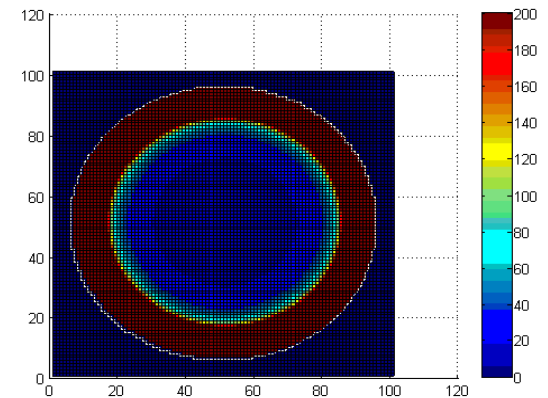
## Hertz



## Error Percent

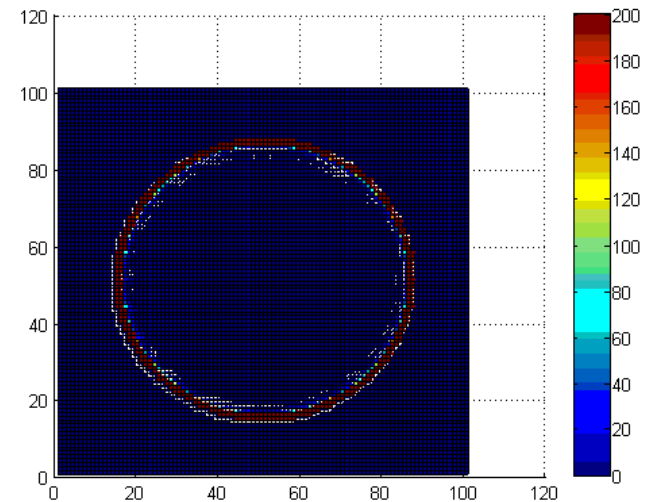
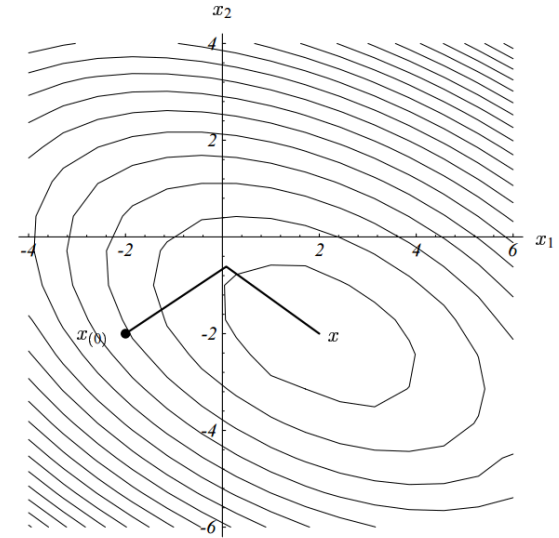


## Error Percent



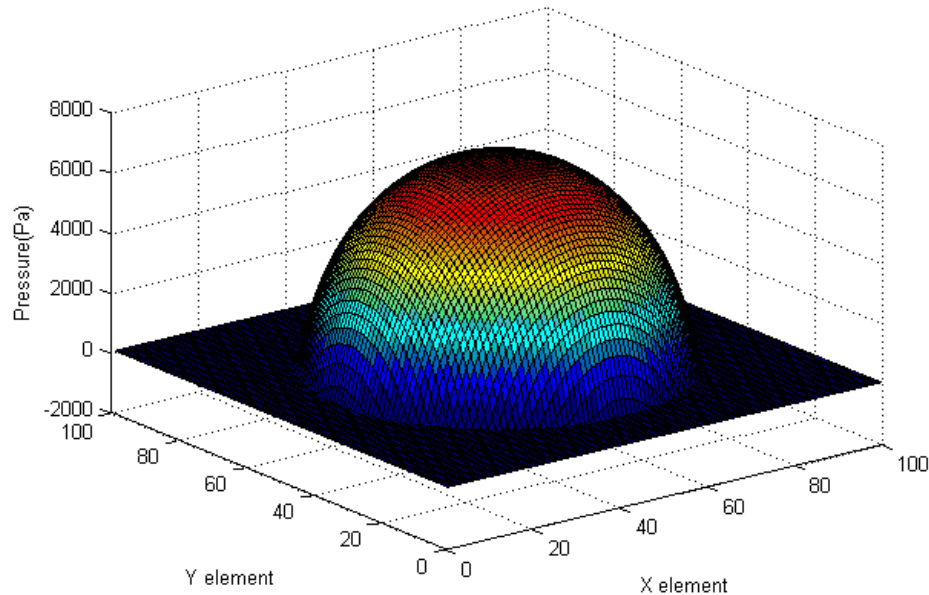
# Improving upon Hu model

- Hu's constrained CGM method was replaced by a constrained *non-linear* CGM with a Newton Raphson line search
- This improves convergence (as shown by Schewchuk (1993)) and accuracy



# NL-CGM Results: Circular & Line Contacts

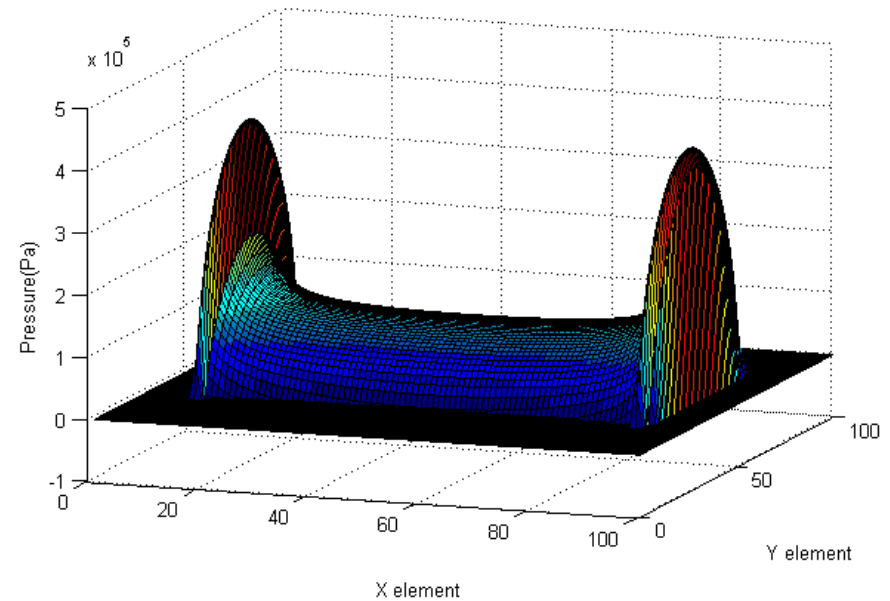
## Pin on Disk



**Numerical error at center element as compared to Hertzian Solution**

Winkler	Hu	NL-CGM
100.14%	18.05%	.35%

## Cylinder

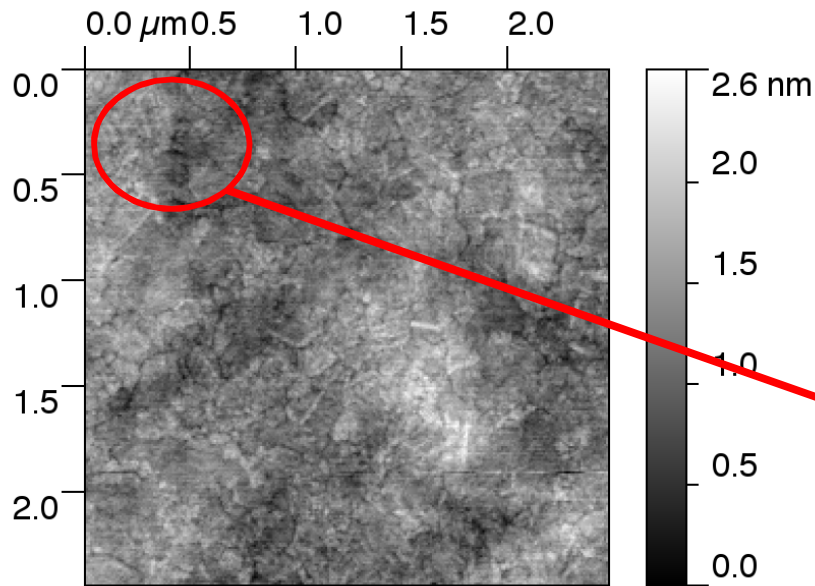


**Numerical error at center element as compared to Hertzian Solution**

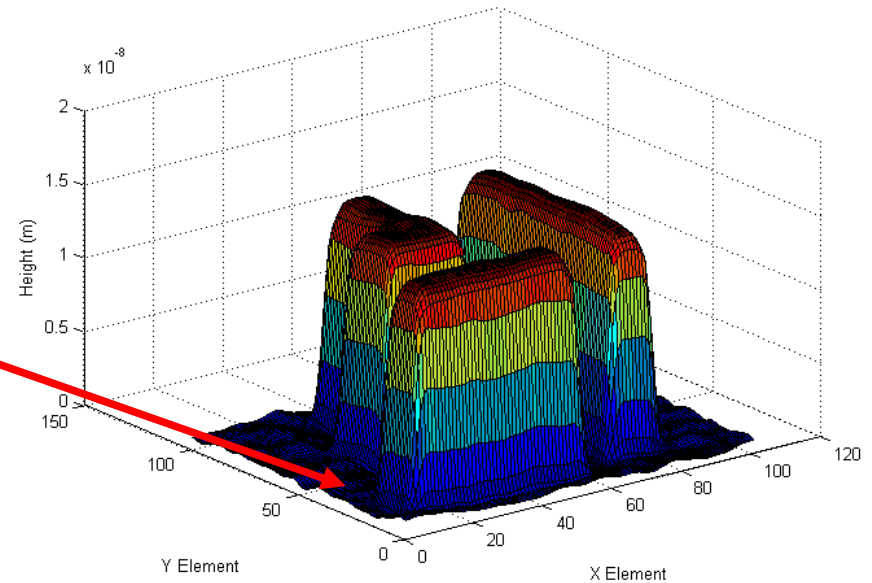
Winkler	Hu	NL-CGM
64.7%	NA	2.56%

# Introducing Metrology Data: Real Surface

AFM Data

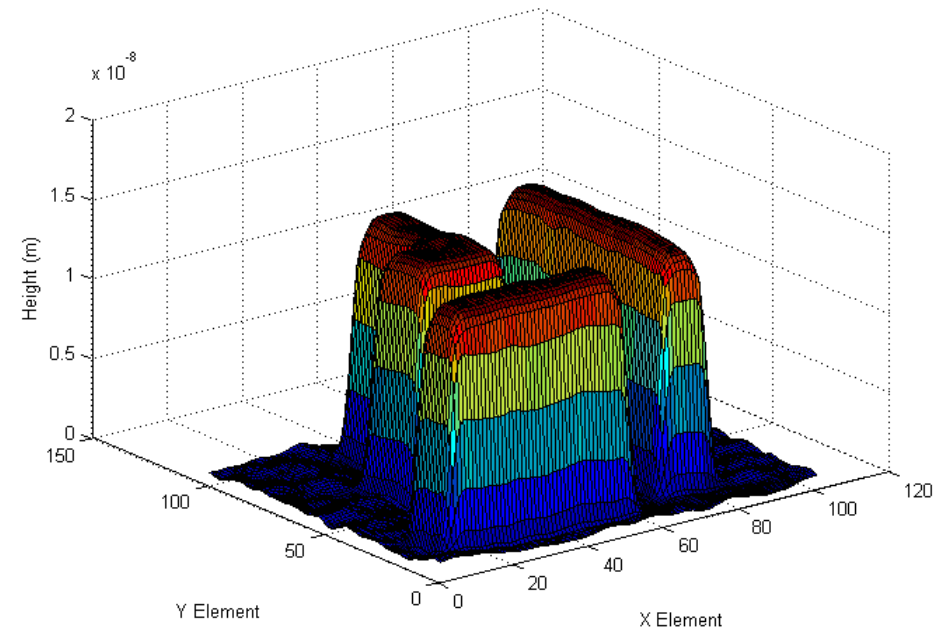
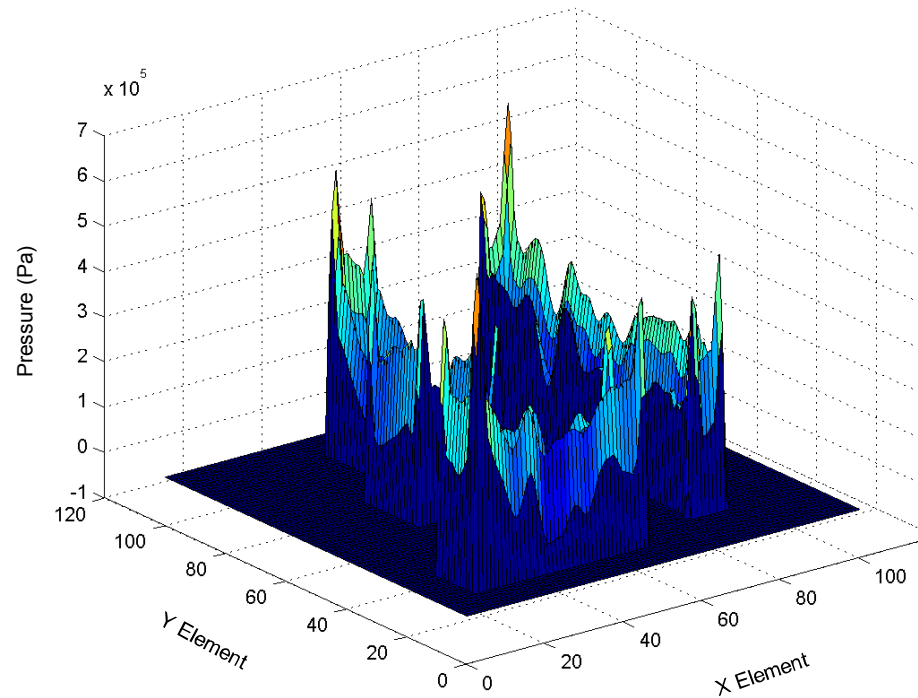


Raised surface prior to CMP using AFM data



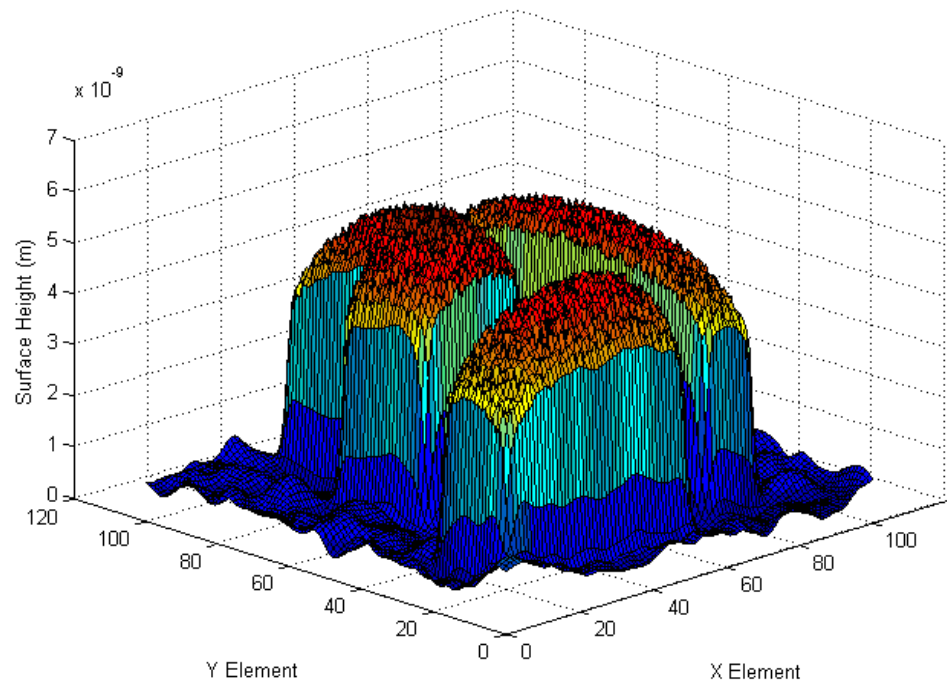
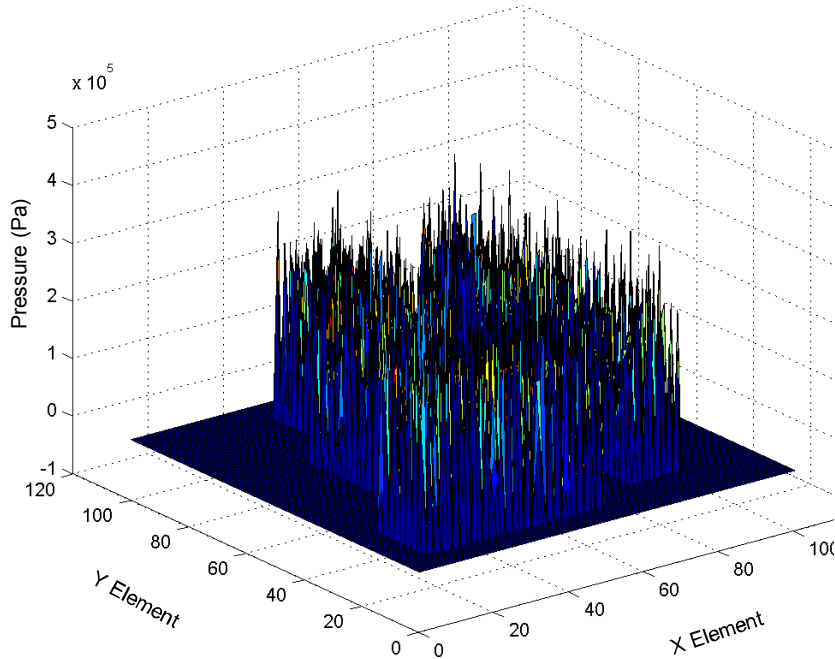
# NL-CGM Results: Extending to IC Feature Geometries

<b>Average Load</b>	5 psi	<b>Relative velocity</b>	.3 m/s
<b>Simulation time step</b>	.01s	<b>Preston coefficient</b>	60 MPa <sup>-1</sup>
<b>Element Size</b>	10nm x 10nm	<b>Error tolerance</b>	1%



# NL-CGM Results: Extending to IC Feature Geometries

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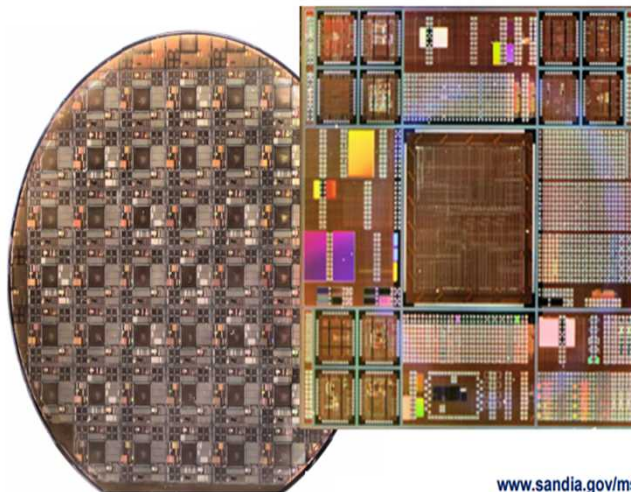
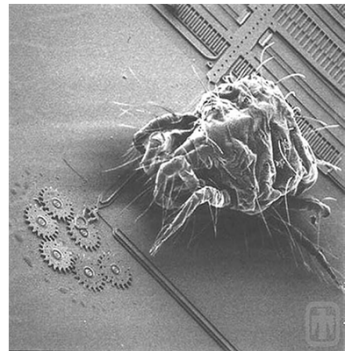
# SNL: MESA Complex

## Silicon Fab

Trusted Rad-Hard application specific integrated circuits (ASIC)  
Micro Electromechanical Systems (MEMS)  
Photonics & more...

## Micro Fab

III-V Compound Semiconductor Devices  
Power Electronics  
Advanced packaging



[www.sandia.gov/mstc](http://www.sandia.gov/mstc)

## IR Imagers for Remote Sensing



- GaSb-based MWIR/LWIR detector arrays for large-format FPAs
- 10 $\mu$ m indium bump bonding, underfill, thinning, AR coating
- hybridization to silicon ROICs with >99.99% interconnect yield

# Advanced packaging

More functionality, Less Power, Faster performance.... More complexity

Failure analysis requires precise removal layer by layer

Stresses need to be considered at a micro scale

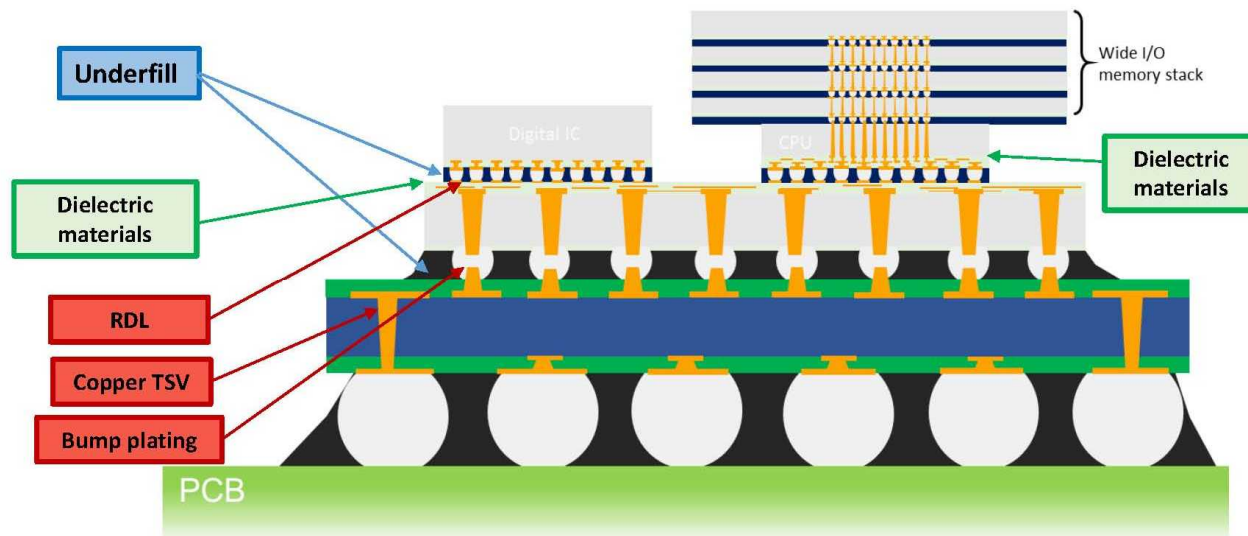
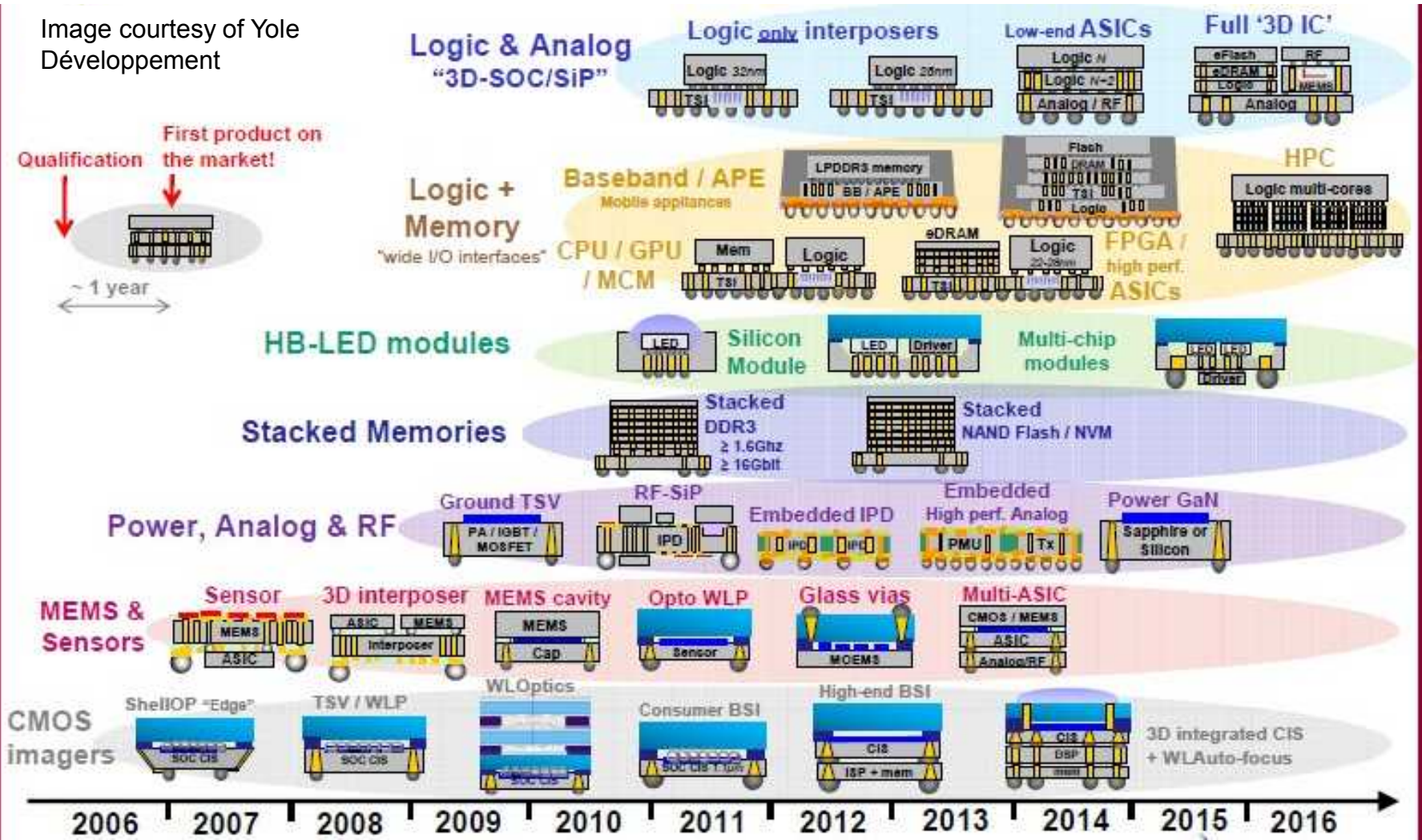


Image courtesy of Yole Développement

# Advanced Packaging strategies

Image courtesy of Yole Développement

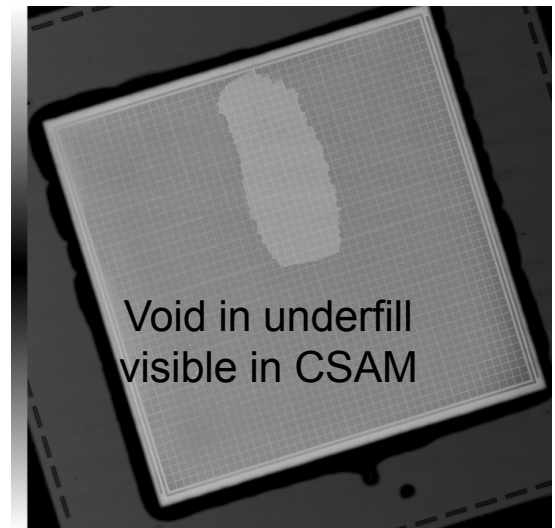
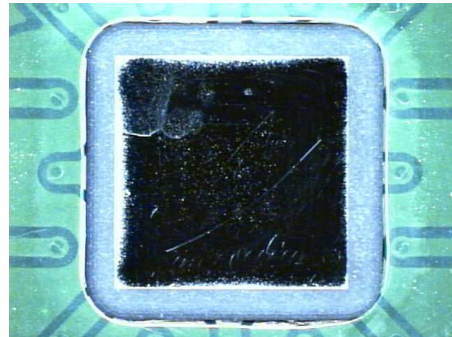
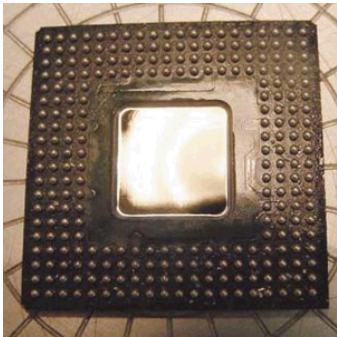
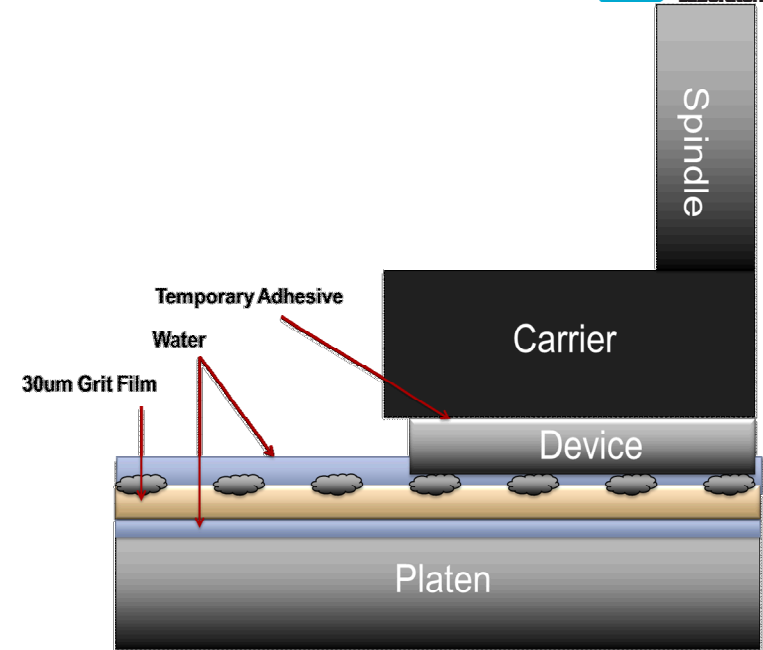


# Device Thinning

Devices are often thinned for failure analysis or manufacturing purposes on a CMP-like tool

Challenges to consistency include:

- Debris affects removal rate and selectivity
- Water-Film-Water stack
- Film Slippage



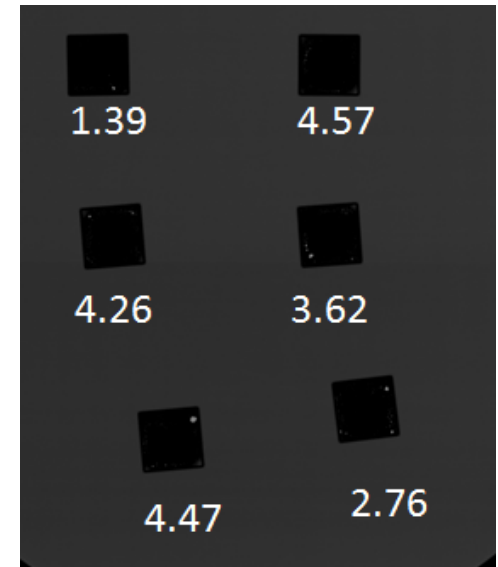
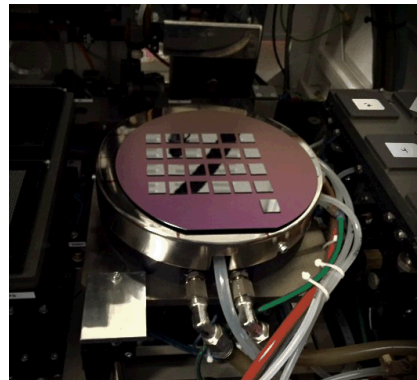
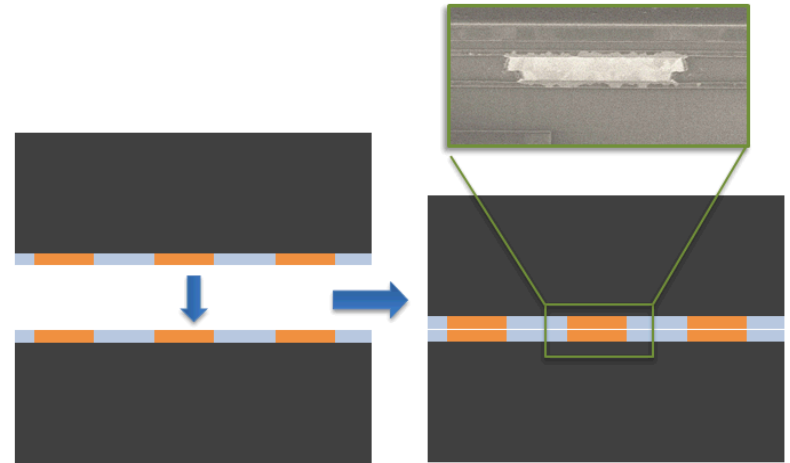
# Wafer Bonding

Two silicon wafers, or die can be bonded at low temperatures and form a hermetic seal

The bonded wafers/die can have functional patterned interconnect with the right materials and minimal dishing

## Challenges:

- Contact points affect the bond quality
- Grain boundaries in metals
- Non Selective CMP



Percent Area uncontacted under each die

# Conclusion

- Presented a high fidelity and accuracy CMP-focused contact mechanics approach capable of resolving wear and nano-topography
- IC fabrication is evolving to include extremely complex 3D structures
- Plenty of niche areas which could benefit from robust contact mechanics frameworks

# Acknowledgements

- Prof. C. Fred Higgs III
- Prof. Shawn Blanton (ACTL)
- Prof. Shawn Litster (TPES)
  
- Sandia 1740 Group,
- MesaFab CMP Team
- HTS Team
- Dr. Sara Jensen
- Dr. Adam Jones

THANK YOU

# Extra Slides

# Contact Mechanics Implementation

- Direct matrix multiplication is too expensive.

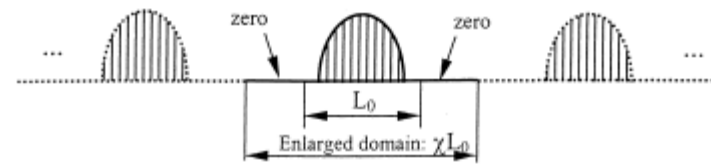
$$u = C \cdot p$$

- Implemented through a memory saving Fast Fourier Transform (FFT) approach.

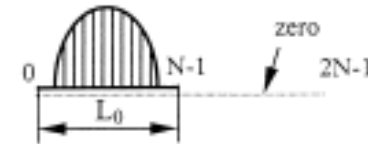
- In order to meet periodic and infinite domain conditions of FFT, zero padding and domain wrap around are employed

- Liu et al. 2000

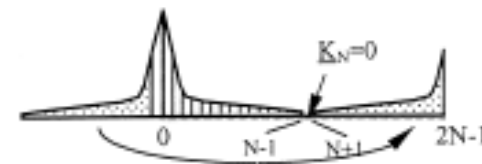
Extended Periodic Domain



Zero Padding

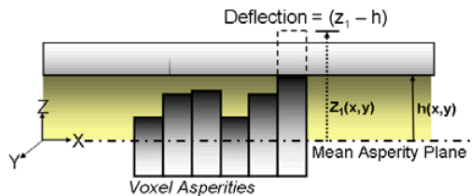


Wrap Around



# Three Contact Model Comparison

## Winkler

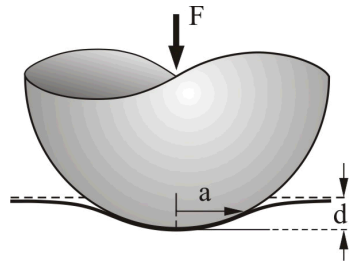


$$\Delta H_{x,y} = \frac{\sigma_{x,y}}{E} \frac{(1-2\nu)(1+\nu)}{(1-\nu)} t$$

$$\sigma_{x,y} = \frac{E_v}{t} \Delta H_{x,y}$$

$$\frac{E_v}{t} = 1.35 \frac{E^*}{a}$$

## Hertzian



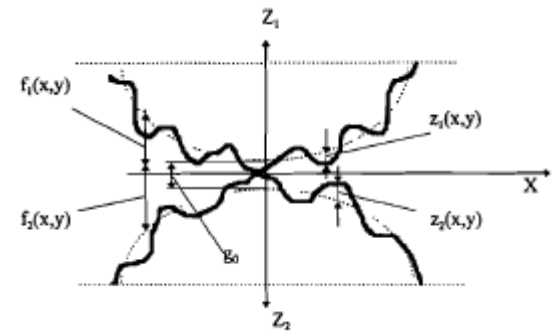
$$a = \left( \frac{3WR}{4E^*} \right)^{1/3}$$

$$\delta = \frac{a^2}{R}$$

$$\sigma = \sigma_0 \left\{ 1 - \left( \frac{r}{a} \right)^2 \right\}^{.5}$$

$$\sigma_0 = \frac{3W}{2\pi a^2}$$

## Elastic halfspace with FFT, and constrained CGM (Hu et. al 1999)



$$\text{Minimize } F(\sigma) = \hat{g}\sigma + \frac{1}{2} \sigma C \sigma$$

$$\text{subject to : } \sigma \geq 0$$

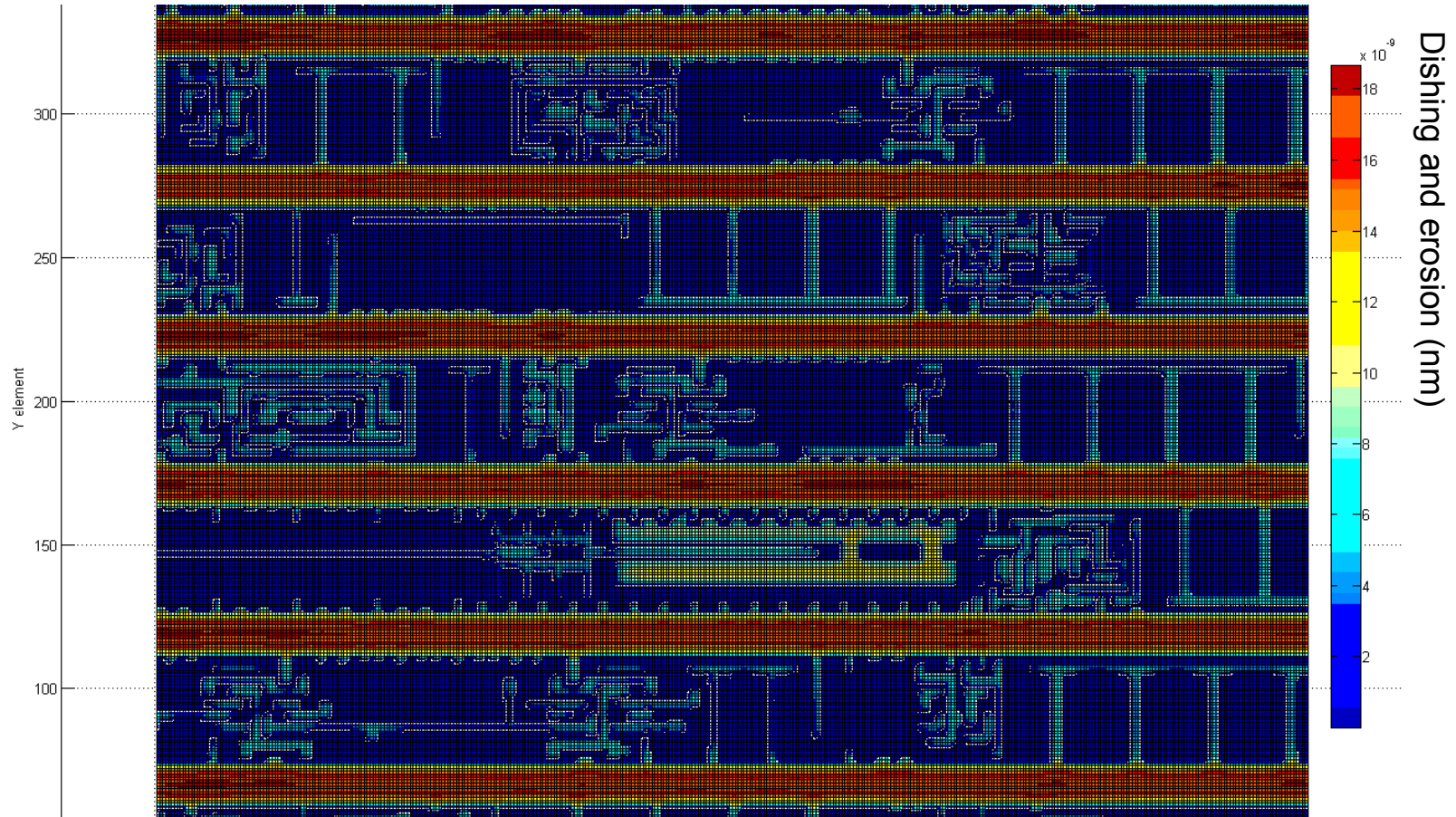
$$\text{KKT condition: } \begin{array}{l} \sigma_{x,y} = 0 \quad \frac{\partial F}{\partial \sigma} \geq 0 \\ \sigma_{x,y} > 0 \quad \frac{\partial F}{\partial \sigma} = 0 \end{array}$$

$$\Rightarrow \frac{\partial F}{\partial \sigma} = \bar{g} + C\sigma = g$$

# Non-Linear CGM

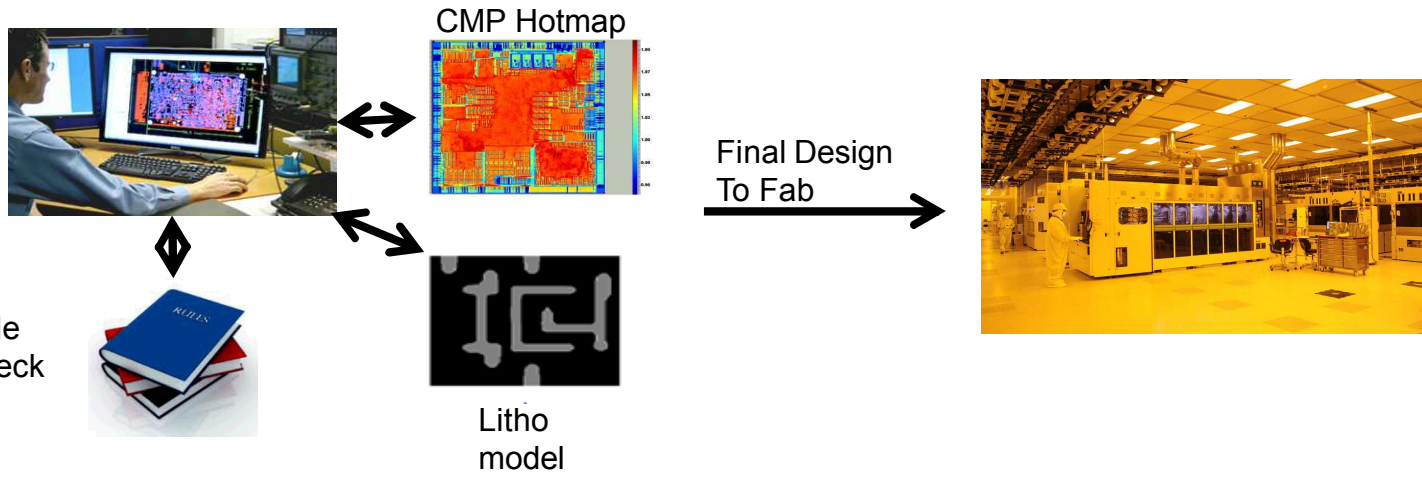
```
 $i \leftarrow 0$   
 $k \leftarrow 0$   
 $r \leftarrow -f'(x)$   
 $d \leftarrow r$   
 $\delta_{new} \leftarrow r^T r$   
 $\delta_0 \leftarrow \delta_{new}$   
While  $i < i_{max}$  and  $\delta_{new} > \epsilon^2 \delta_0$  do  
   $j \leftarrow 0$   
   $\delta_d \leftarrow d^T d$   
  Do  
     $\alpha \leftarrow -\frac{[f'(x)]^T d}{d^T f''(x) d}$   
     $x \leftarrow x + \alpha d$   
     $j \leftarrow j + 1$   
  while  $j < j_{max}$  and  $\alpha^2 \delta_d > \epsilon^2$   
     $r \leftarrow -f'(x)$   
     $\delta_{old} \leftarrow \delta_{new}$   
     $\delta_{new} \leftarrow r^T r$   
     $\beta \leftarrow \frac{\delta_{new}}{\delta_{old}}$   
     $d \leftarrow r + \beta d$   
     $k \leftarrow k + 1$   
  If  $k = n$  or  $r^T d \leq 0$   
     $d \leftarrow r$   
     $k \leftarrow 0$   
 $i \leftarrow i + 1$ 
```

# CMP on Post litho M1 (10s simulation)

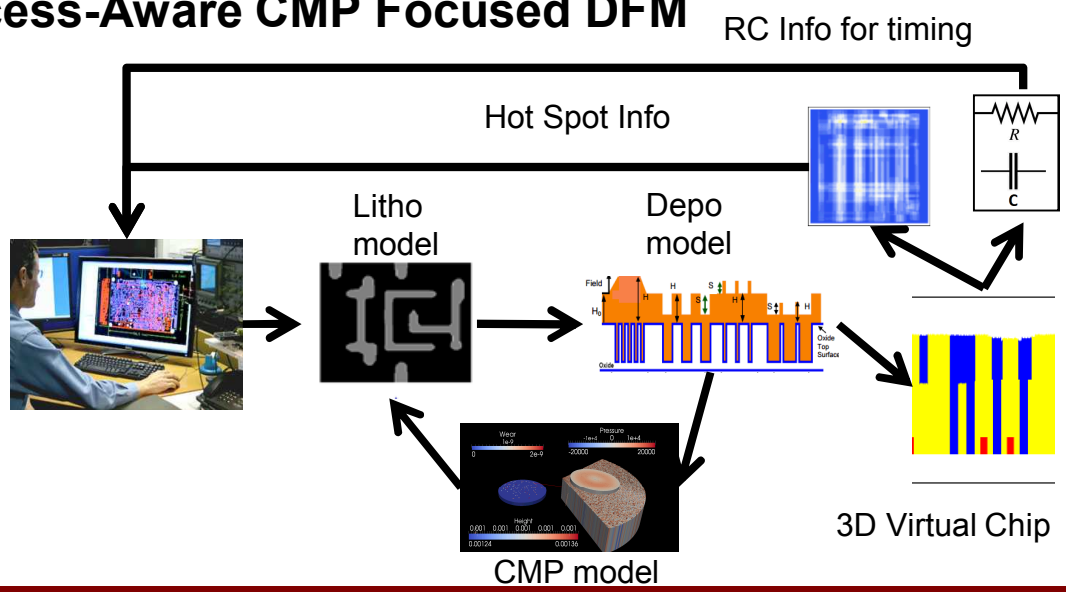


# Process-Aware CMP-Focused DFM framework

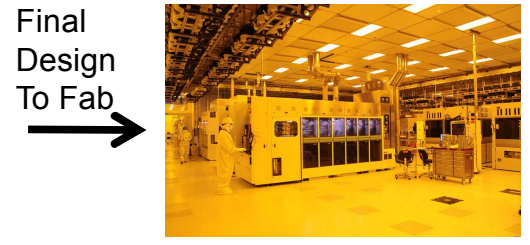
## Current DFM (segregated)



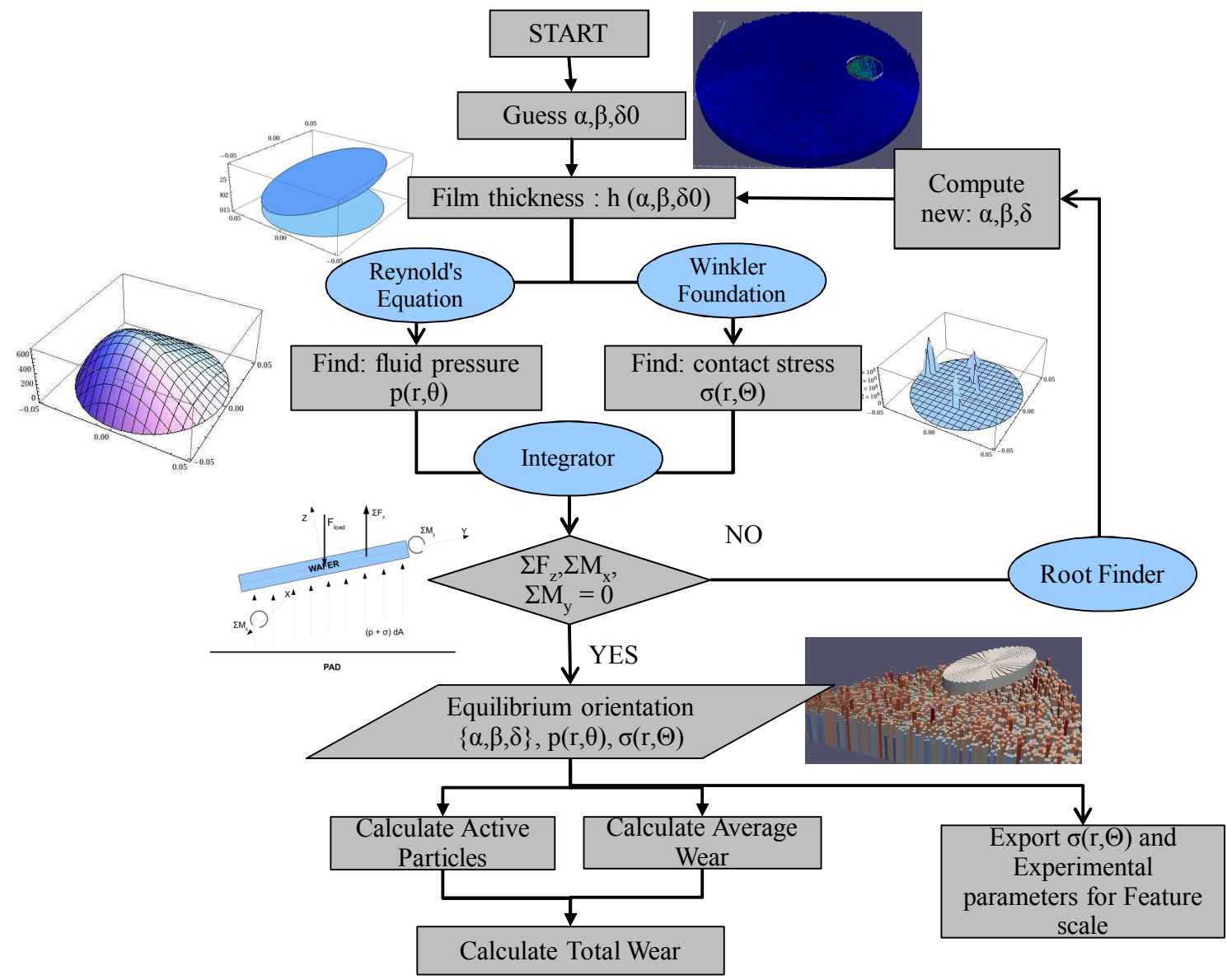
## Process-Aware CMP Focused DFM



**Useful to:**  
Chip Design, Manufacturing & Test Engineers



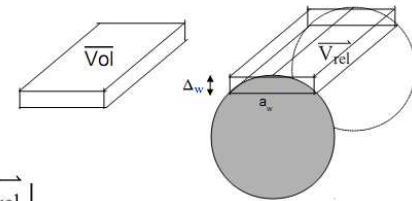
# Wafer-Scale Topography Simulation Flowchart (PAML-lite)



# Feature-Scale Wear Modeling of CMP

- Soft pad model given by Luo and Dornfeld (2003) implemented.
- Wear depends on:
  - Number of active particles (Particles participating in the wear event)
  - Average wear (Material removed by a average active particle)
  - Local Contact Stress
  - Local Material Hardness

## Average Wear per Particle



- Abrasive wear,

$$\overline{\text{Vol}} = \Delta_w a_w |\overline{V}_{\text{rel}}|$$

$$\Delta_w = \sqrt{\frac{2F}{\pi H_w}} |\overline{V}_{\text{rel}}| = |\overline{V}_p - \overline{V}_w|$$

$$F = \sigma * \pi x^2 \quad a_w = \frac{2F}{\pi x_{\text{avg-a}} H_w}$$


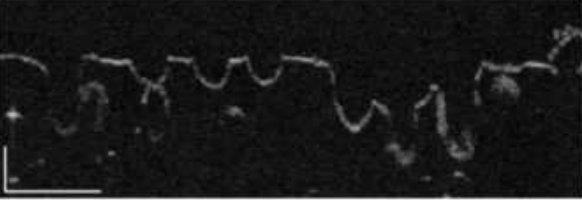
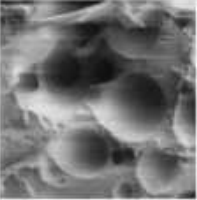

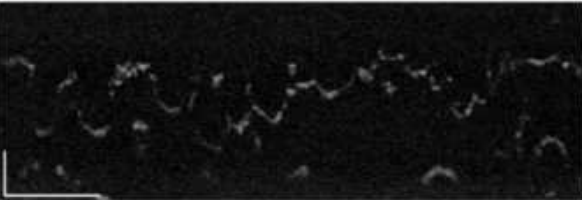
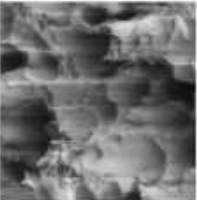
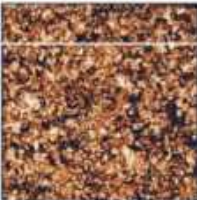
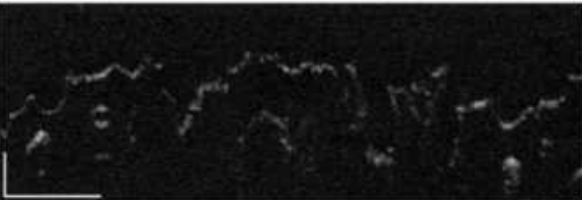
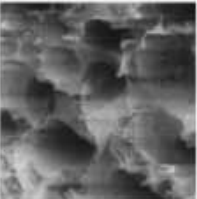

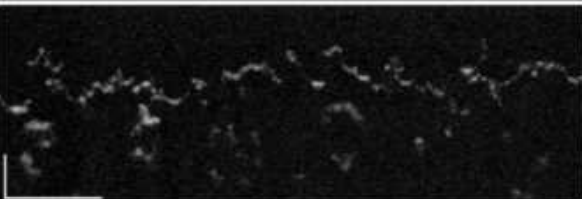
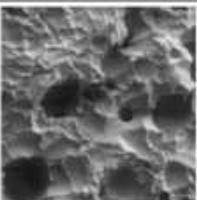


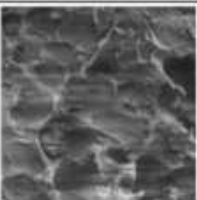
Reduces to the following equation

$$\overline{\text{Vol}} = \frac{1}{2\sqrt{2}} x_{\text{avg-a}}^2 \left(\frac{\sigma}{H_w}\right)^{3/2} V_{\text{rel}}$$

## MRR Equation at Feature Scale:

$$\frac{dh_{\text{vox}}}{dt} = \frac{1}{2\sqrt{2}} x_{\text{avg-a}}^2 \left(\frac{\sigma(x, y)}{H_w(x, y)}\right)^{3/2} V_{\text{rel}}(x, y) \frac{N_{\text{act}}(x, y)}{A_{\text{vox}}}$$

# CMP Pad Magnification

Pad usage	3-D OCT image of pad surface (Top view)	Cross-sectional OCT image of pad (white line in 3D OCT image)	SEM image (500X)
(a) Unpolished new pad			
(b) 68 wafers polished pad			
(c) 139 wafers polished pad			
(d) 178 wafers polished pad			
(e) End of life pad			

# Modeling Parameters

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## Pad Properties

Model Simulated	IC 1000
Hardness	5.0 MPa
Elastic Modulus	12 MPa
Asperity Distribution	Random Gaussian
Pad Thickness	1.3 mm
Roughness	10 $\mu\text{m}$
Poisson's Ratio	0.4

## Wafer Properties

Hardness	2.0 Gpa (SiO <sub>2</sub> ), .38 Gpa (Cu)
Elastic Modulus	110 GPa
Poisson's Ratio	0.16

## Slurry Properties

Particle Material	Silica
Particle Density	2000 kg / m <sup>3</sup>
Particle Size Distribution	Gaussian
Mean Particle Radius	150 nm
Standard Deviation of Particle Radius	15 nm
Fluid Density	1000 kg / m <sup>3</sup>
Fluid Viscosity	0.001 Pa - s
Concentration	2% (wt/wt)

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## Operating Parameters

Load	4psi
Wafer RPM	50
Pad RPM	90
Layout	3x5 SRAM Array
Layout Size	1.5 $\mu\text{m}^2$

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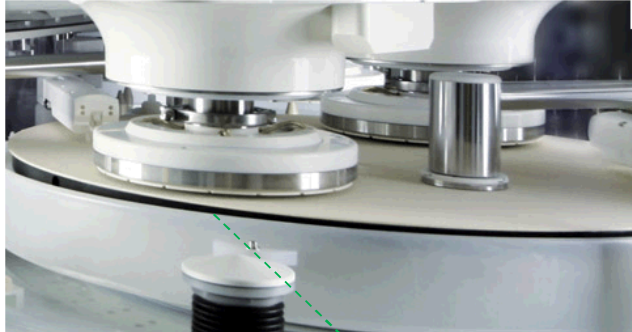
# CMP Modeling: Literature Across the Scales

## Select CMP Models

<b>Wafer Scale</b>	<b>Die Scale</b>	<b>Feature Scale</b>	<b>Multi Scale</b>
Sundararajan et al. (1999) Zhao & Chang (2001) Luo & Dornfeld (2001) Shan et al. (2001) Fu et al. (2001) Higgs et al. (2005) Jin et al. (2005) Beschoner et al. (2009) Srivastava & Higgs (2013) Sierra-Suarez et al. (2013)	Stine et al. (1997) Tugbawa et al. (1999) Ouyang et al. (2000) Ouma et al. (2002) Luo & Dornfeld(2003) Xie et al. (2003)	Runnels et al (1994) Chekina et al. (2000) Zhao et al. (2003) Vlassak (2004) Saxena et al. (2004) Terrell & Higgs(2009) Comes et al. (2010)	Seok et al. (2003) Tripathi et al. (2007) Wang et al. (2007) Kasai & Bushan (2008) Sierra-Suarez et al. (2013)

# Wafer-Scale Model: PAML-lite

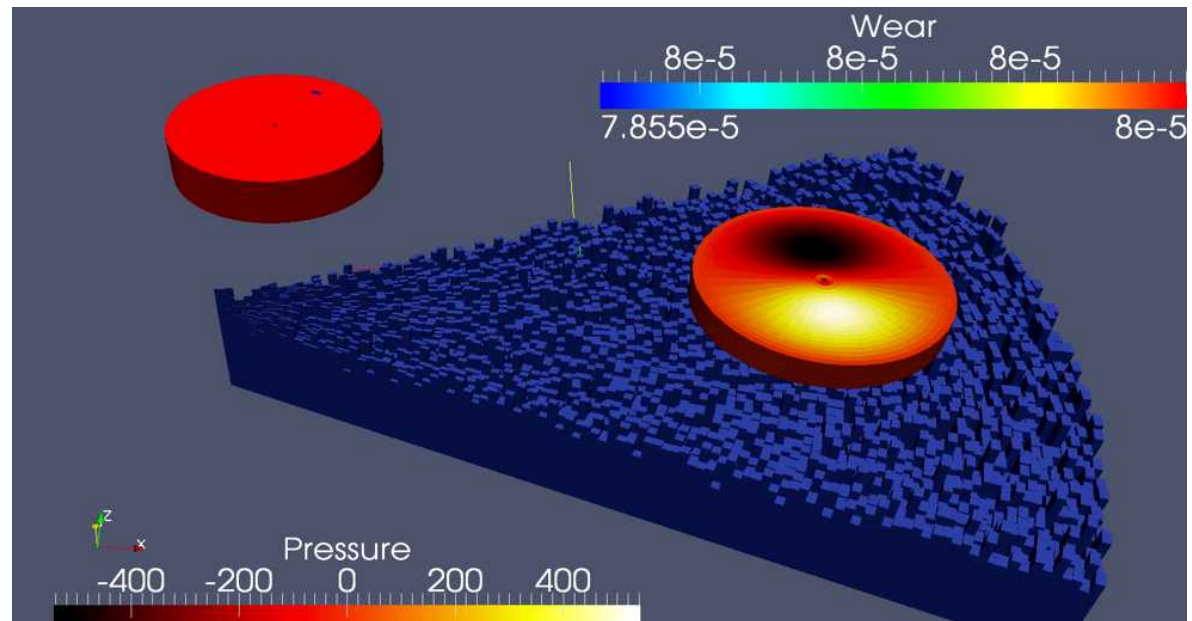
## *Application:* CMP



## *Virtual CMP*

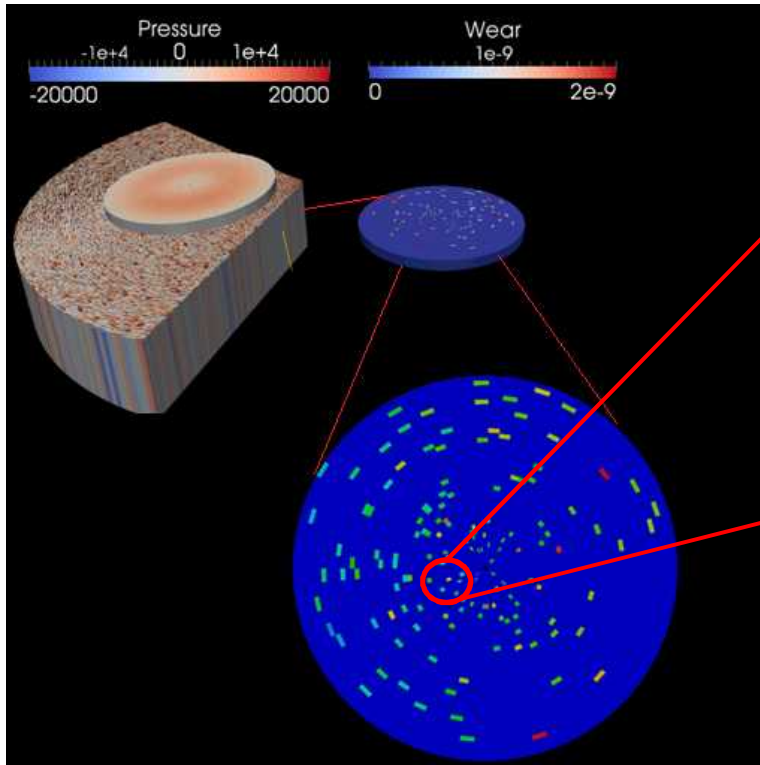
*(Multiphysics fluid structure interaction & Wear)*

- Wafer-scale mixed lubrication model from Srivastava & Higgs (2013)
- The evolution of wear, fluid pressure, and contact stress is monitored

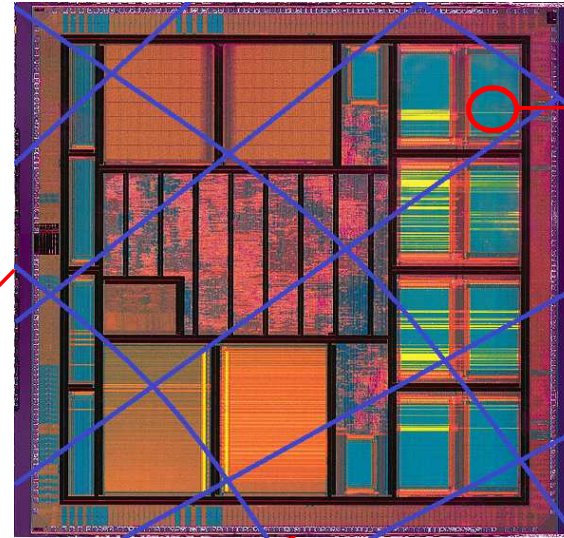


# CMP Simulation: From Wafer to Layout Features

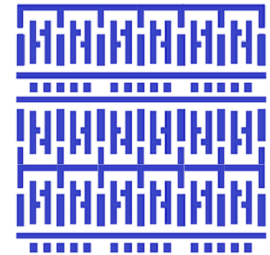
## Wafer-Scale Simulation



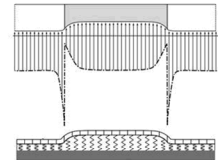
## Die View



## SRAM Array Metal 1 Layout



## Simulate Local Wear



## Resulting Local Surface

