ATPESC, St. Charles, Aug. 13, 2015

Computational Science and Cinema

Marius Stan

Argonne NATIONAL LABORATORY

SONY PICTURES TELEVISION

Breaking Bad

facebook Bogdan's Eyebrows

Blog entries:

"Bogdan doesn't look like a happy man. Plus, he's fairly old -- 60's, probably."

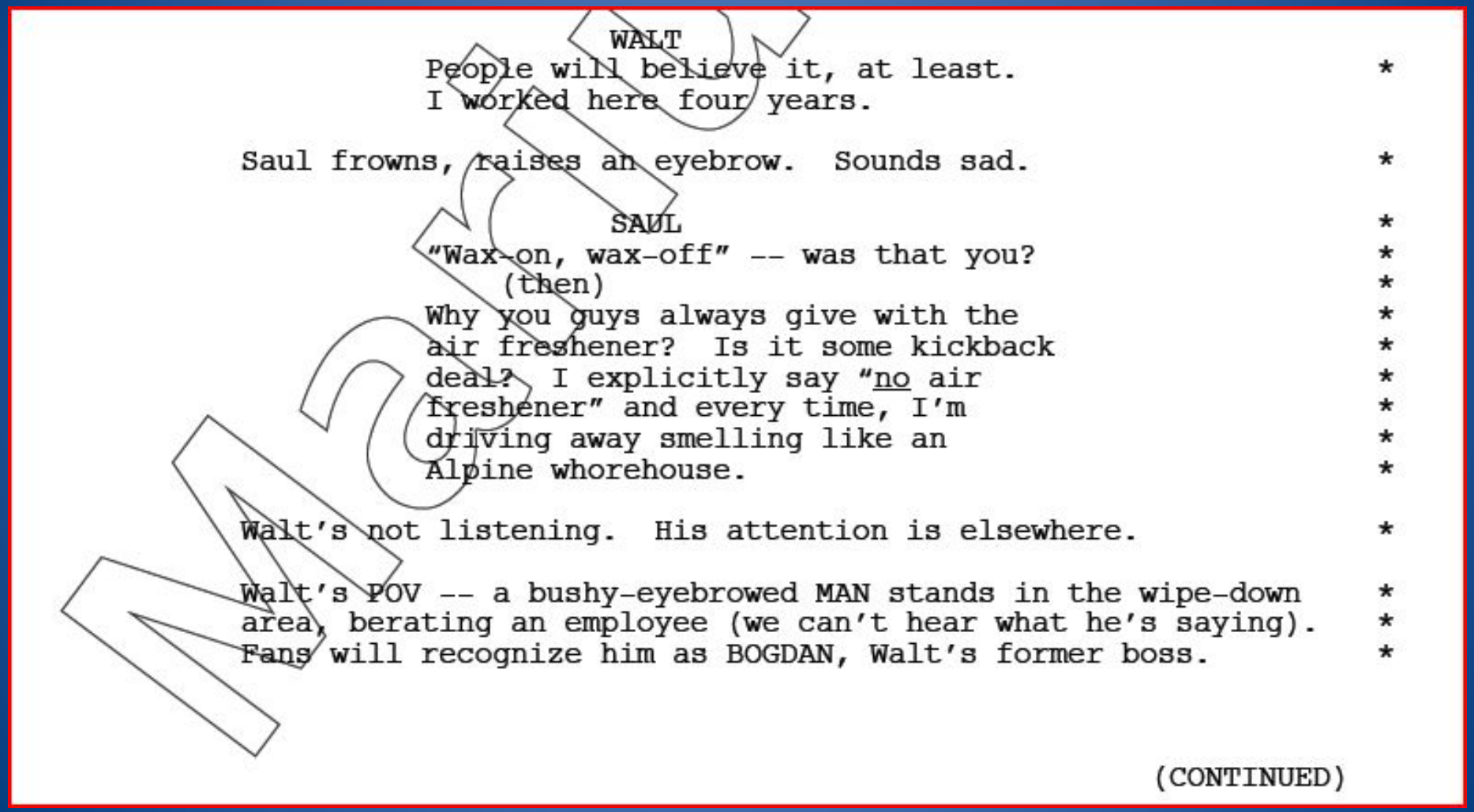
"He has a tumor."

"His wife wants to move back to the old country."

"His mistress needs a new car."

A good script

Breaking Bad, Ep. 311, “Abiquiu”



WALT
People will believe it, at least. *
I worked here four years.

Saul frowns, raises an eyebrow. Sounds sad. *

SAUL *
“Wax-on, wax-off” -- was that you? *
(then) *
Why you guys always give with the *
air freshener? Is it some kickback *
deal? I explicitly say “no air *
freshener” and every time, I’m *
driving away smelling like an *
Alpine whorehouse. *

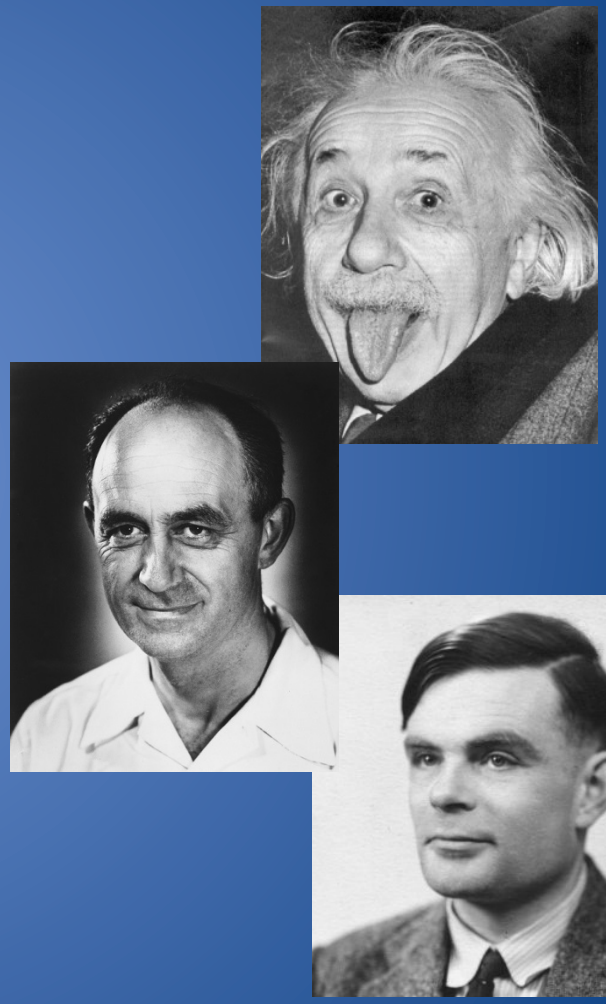
Walt’s not listening. His attention is elsewhere. *

Walt’s POV -- a bushy-eyebrowed MAN stands in the wipe-down *
area, berating an employee (we can’t hear what he’s saying). *
Fans will recognize him as BOGDAN, Walt’s former boss. *

(CONTINUED)

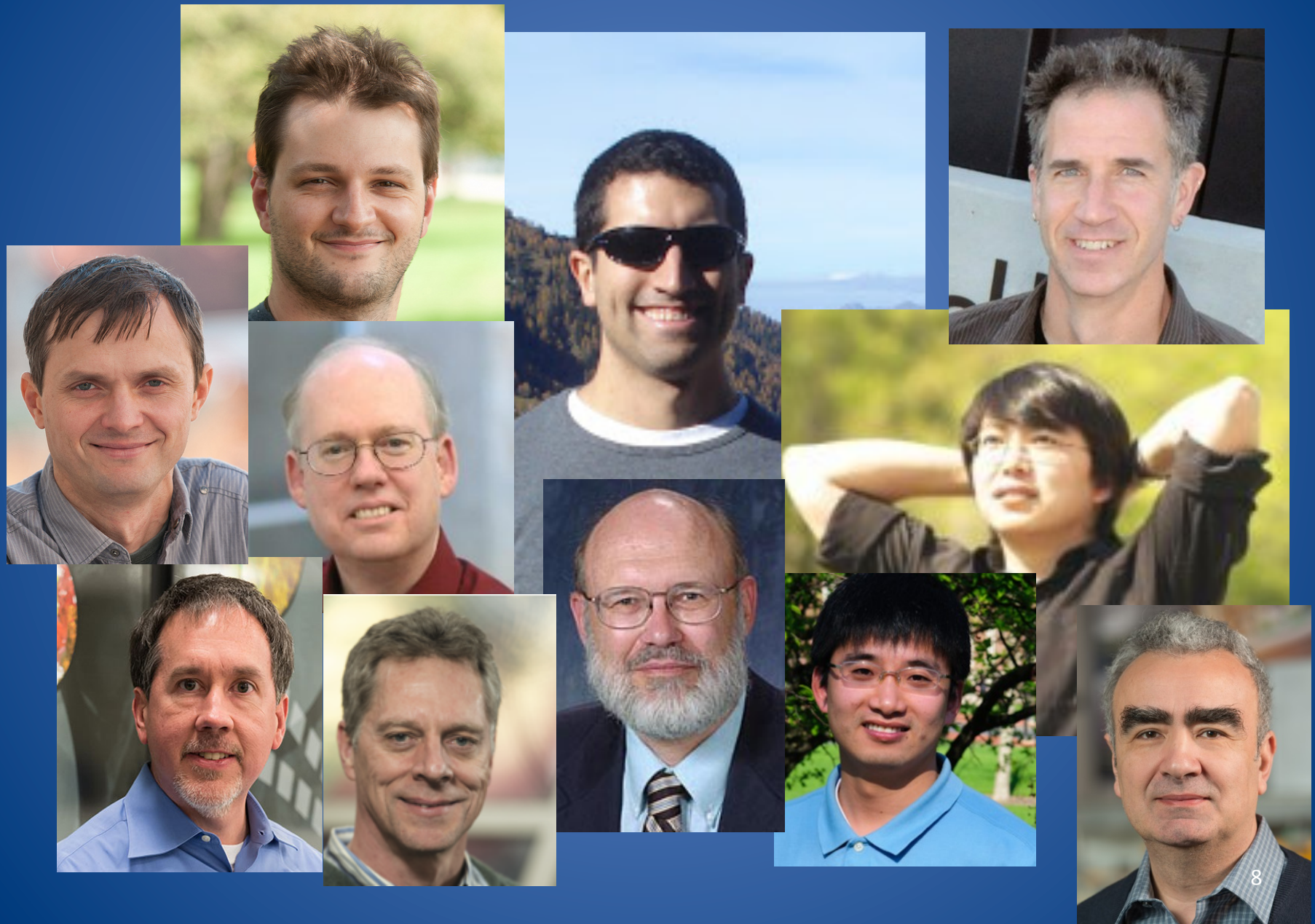
The Scientific Method

- Observation - Question
- Hypothesis
- Model
- Prediction
- Validation
- Communication



A good team

Computational Scientists at Argonne



People

NEAMS
NUCLEAR ENERGY ADVANCED MODELING & SIMULATION PROGRAM

E. Merzari, A. Obabko *et al.*

University of Chicago

M. Wild *et al.*

P. Voorhees, C. Wolverton *et al.*

G. Olson, O. Heinonen *et al.*

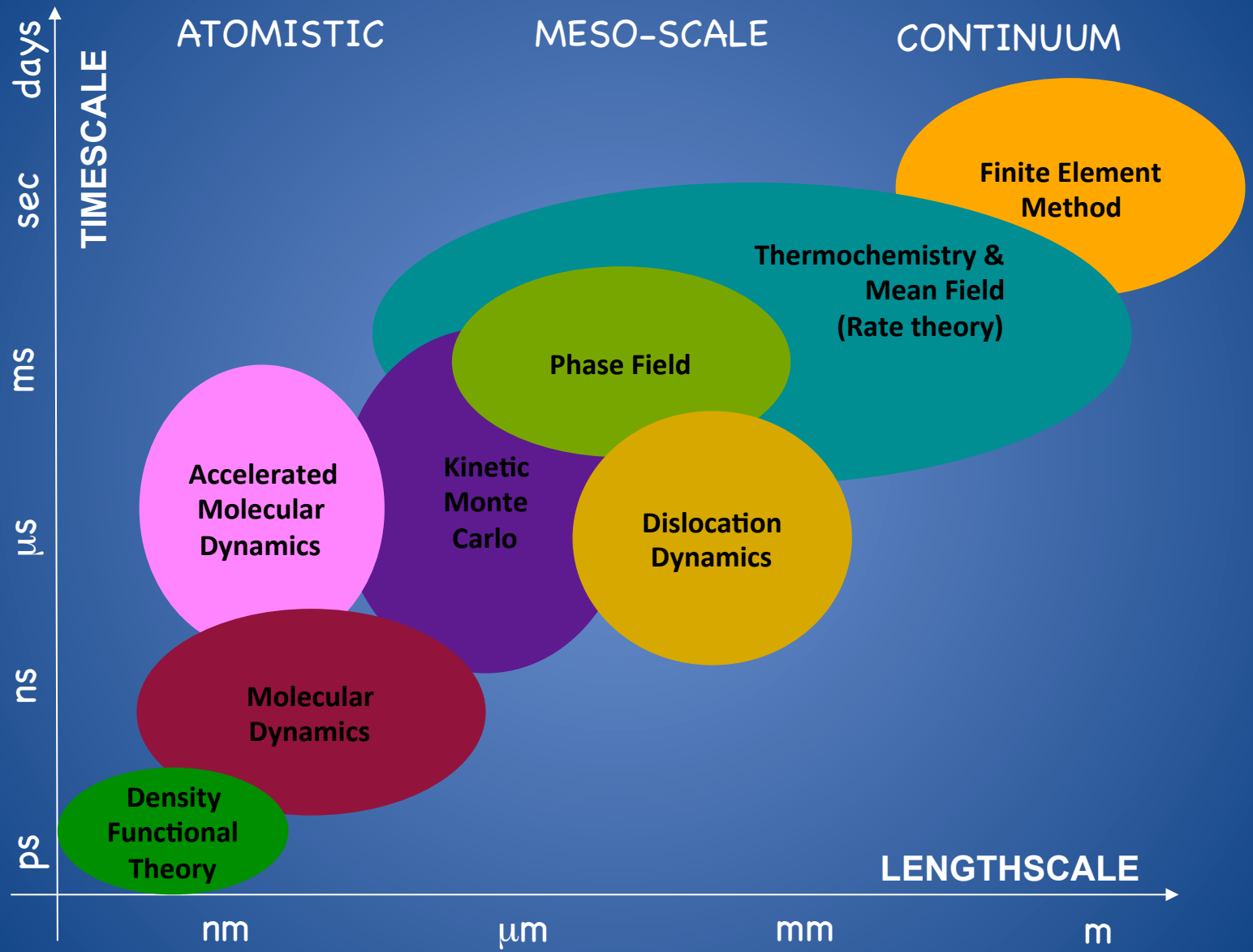
M. Welland, L. Curtiss *et al.*

At the Breaking Bad finale party in Hollywood, CA

Tools

Quiet please.. Roll sound.. Roll Camera.. Action!

Multi-Physics and Multi-Scale

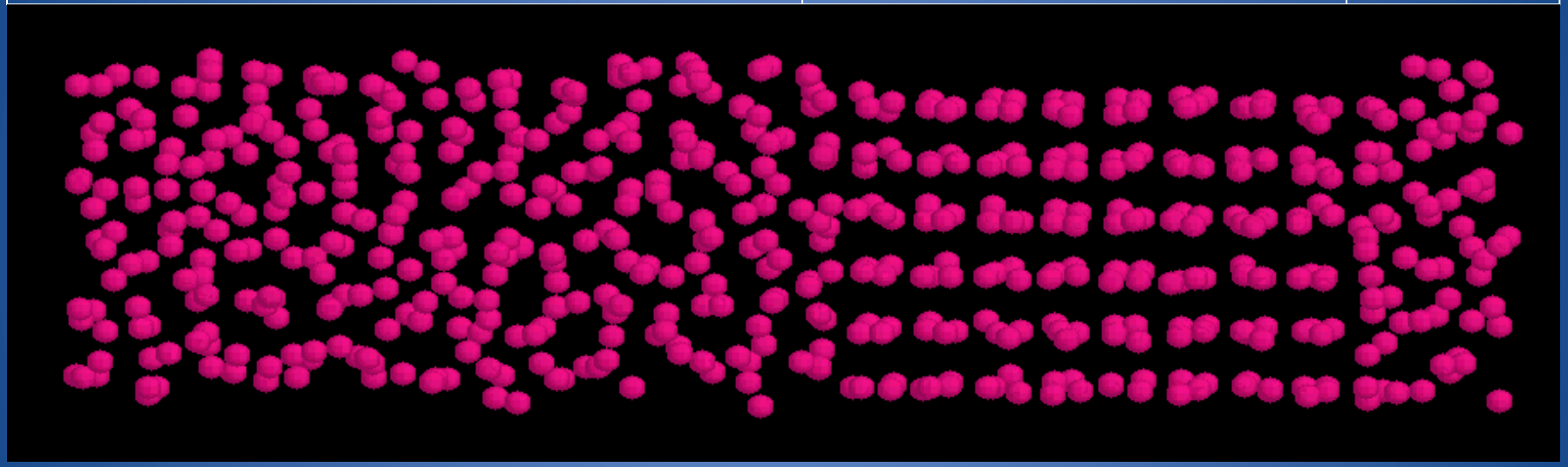


M. Stan, Materials Today, 12 (2009) 20.

Melting of Gallium (Ga)

Melting – atom by atom

Liquid	Solid (A11)	Liquid



M.I. Baskes et al., Phys. Rev. B, 66 (2002) 104
M.I. Baskes and M. Stan, Metal. Mater. Trans., 34A (2003) 435

DON’T TRUST ATOMS

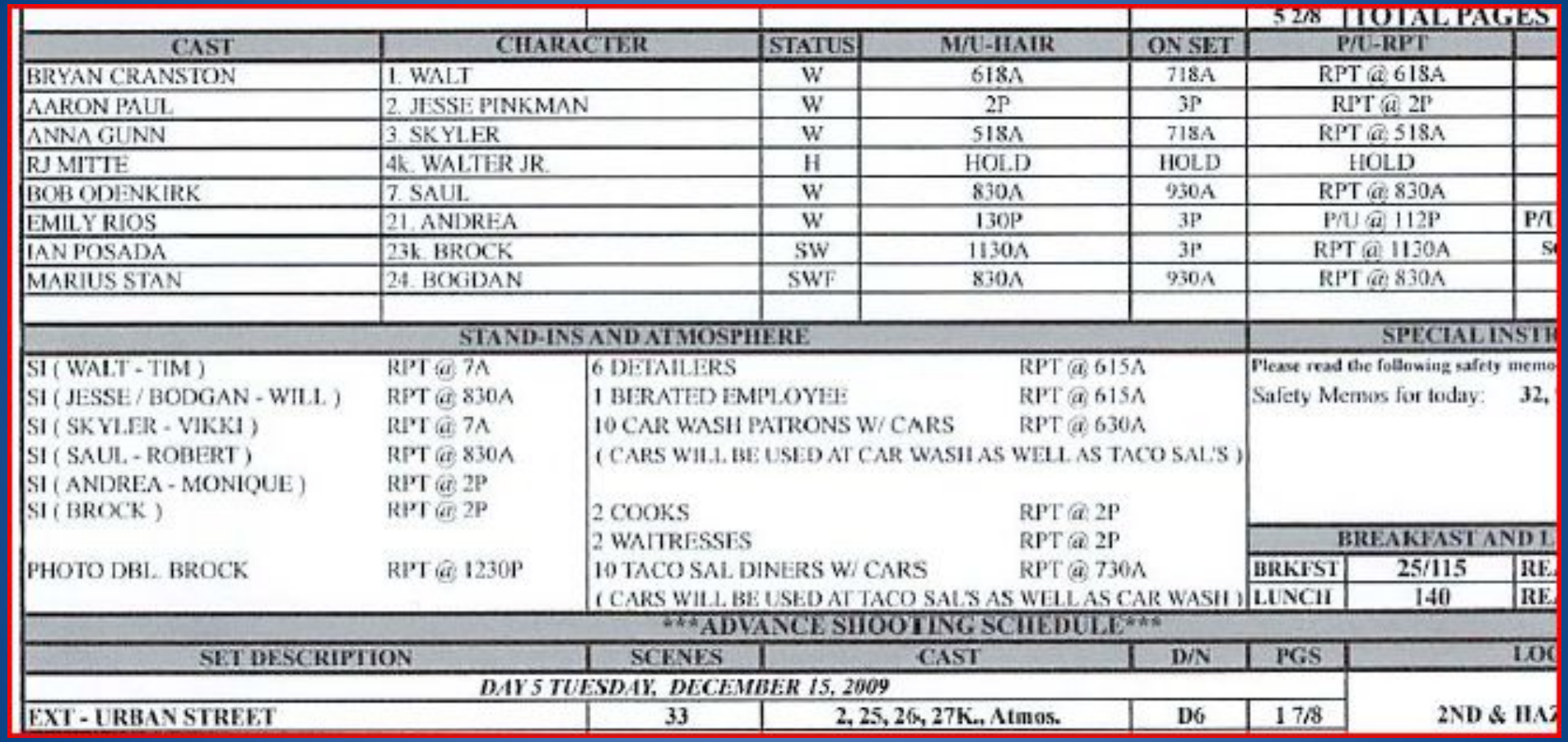
THEY MAKE UP EVERYTHING

T-Shirt

Computers enhance our brain;
they help us understand and predict

Coordination

Cinema: Hair and Makeup at 6:18 AM



5 2/8 TOTAL PAGES

CAST	CHARACTER	STATUS	M/U-HAIR	ON SET	P/U-RPT	
BRYAN CRANSTON	1. WALT	W	618A	718A	RPT @ 618A	
AARON PAUL	2. JESSE PINKMAN	W	2P	3P	RPT @ 2P	
ANNA GUNN	3. SKYLER	W	518A	718A	RPT @ 518A	
RJ MITTE	4k. WALTER JR.	H	HOLD	HOLD	HOLD	
BOB ODENKIRK	7. SAUL	W	830A	930A	RPT @ 830A	
EMILY RIOS	21. ANDREA	W	130P	3P	P/U @ 112P	P/U
IAN POSADA	23k. BROCK	SW	1130A	3P	RPT @ 1130A	S
MARIUS STAN	24. BOGDAN	SWF	830A	930A	RPT @ 830A	

STAND-INS AND ATMOSPHERE				SPECIAL INSTR
SI (WALT - TIM)	RPT @ 7A	6 DETAILERS	RPT @ 615A	Please read the following safety memo
SI (JESSE / BODGAN - WILL)	RPT @ 830A	1 BERATED EMPLOYEE	RPT @ 615A	Safety Memos for today: 32,
SI (SKYLER - VIKKI)	RPT @ 7A	10 CAR WASH PATRONS W/ CARS	RPT @ 630A	
SI (SAUL - ROBERT)	RPT @ 830A	(CARS WILL BE USED AT CAR WASH AS WELL AS TACO SAL'S)		
SI (ANDREA - MONIQUE)	RPT @ 2P			
SI (BROCK)	RPT @ 2P	2 COOKS	RPT @ 2P	
		2 WAITRESSES	RPT @ 2P	BREAKFAST AND L
PHOTO DBL. BROCK	RPT @ 1230P	10 TACO SAL DINERS W/ CARS	RPT @ 730A	BRKFST 25/115 RE
		(CARS WILL BE USED AT TACO SAL'S AS WELL AS CAR WASH)		LUNCH 140 RE

ADVANCE SHOOTING SCHEDULE

SET DESCRIPTION	SCENES	CAST	D/N	PGS	LOC
DAY 5 TUESDAY, DECEMBER 15, 2009					
EXT - URBAN STREET	33	2, 25, 26, 27K., Atmos.	D6	1 7/8	2ND & HAZ

Breaking Bad, Ep. 311, “Abiquiu”

Science: Wrap-up 9:15-9:30 PM

August 13, 2015

Rembrandt Room

3:30 pm - 4:30 pm

Presentation: Globus for Research Data Management

Rembrandt Room

Rachana Ananthakrishnan, Univ. of Chicago

4:30 pm - 5:30 pm

Presentation: Your Turn! Hands on Exercises Kickoff

Rembrandt Room

5:30 pm - 6:30 pm

Dinner Talk: Computational Science and Cinema

Utrillo Dining Room

Marius Stan, ANL

6:30 pm - 9:15 pm

Onwards Hands-on Exercises

Rembrandt Room

9:15 pm - 9:30 pm

Wrap-up

Being creative requires talent

Creating something requires discipline

Money

Twenty million dollars!!!

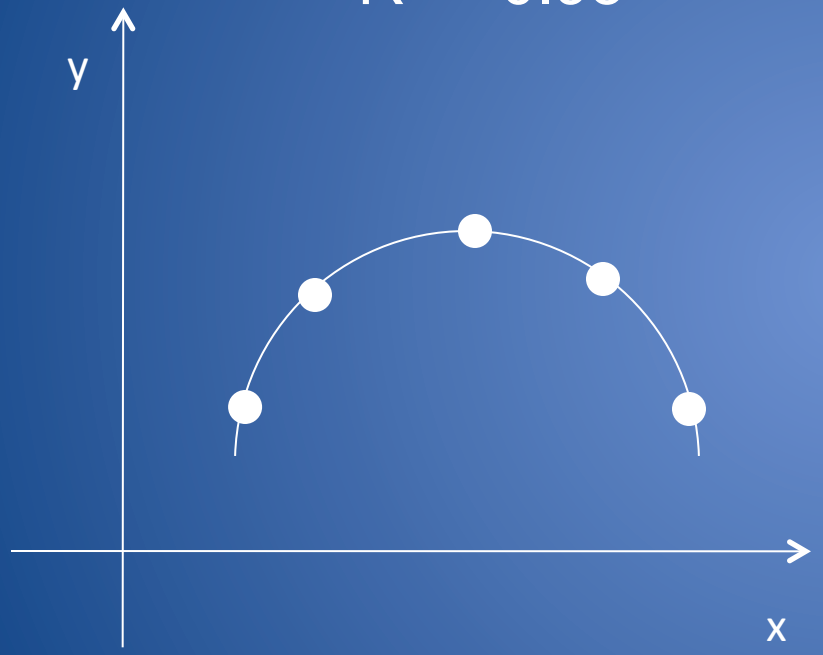
Breaking Bad, Ep. 402, “Thirty-Eight Snub”

Twenty million gigaflops!!!

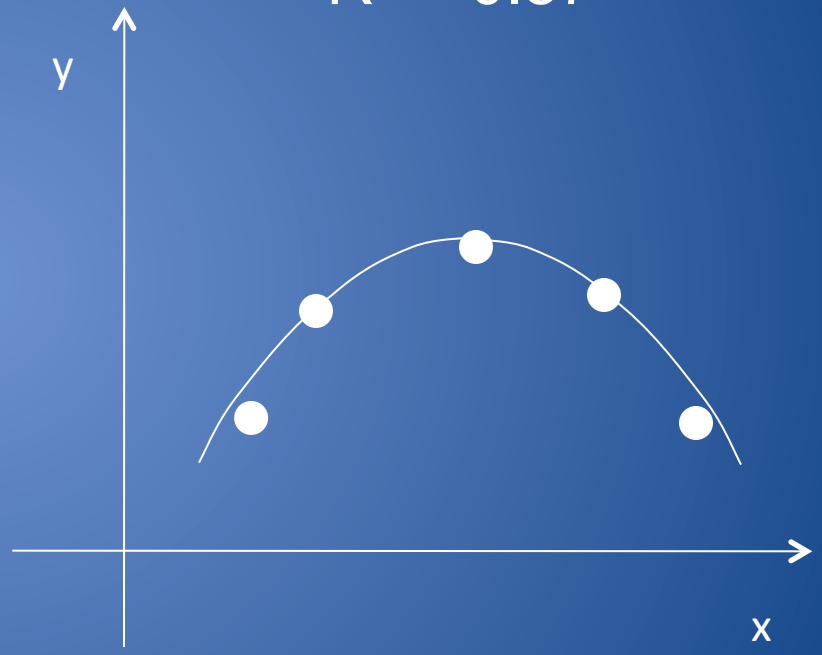
Mid-term test

Object in a gravitational field - observation

Model A
$R^2 = 0.95$

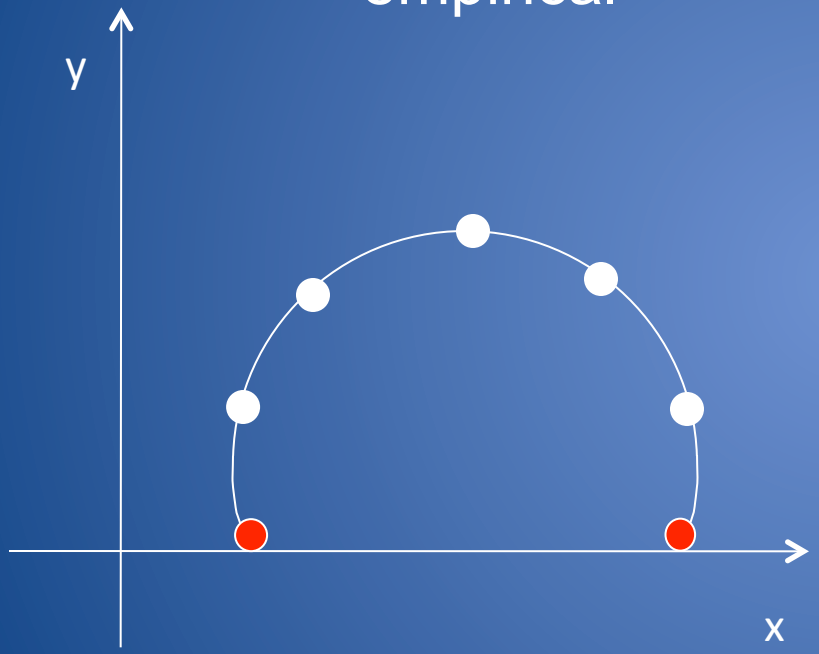


Model B
$R^2 = 0.87$



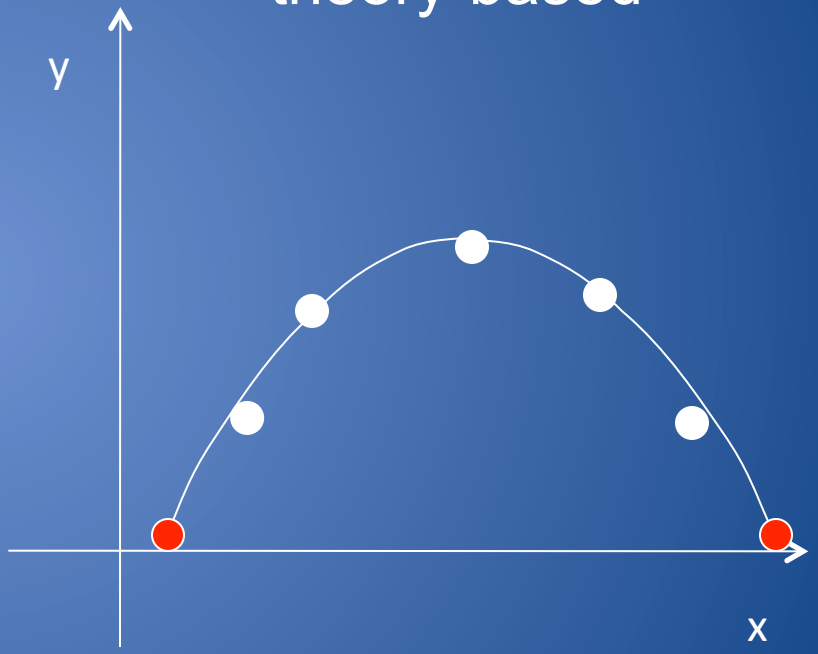
Object in a gravitational field - predictions

Model A
empirical



$$(y-k)^2+(x-h)^2-R^2=0$$

Model B
theory-based



$$4p(y-k)-(x-h)^2=0$$

Theory-based models improve understanding and prediction

But is this correct?

Solution verification

Precision and accuracy

Alien Resurrection, 1997

Creativity

Artists create and communicate
emotions

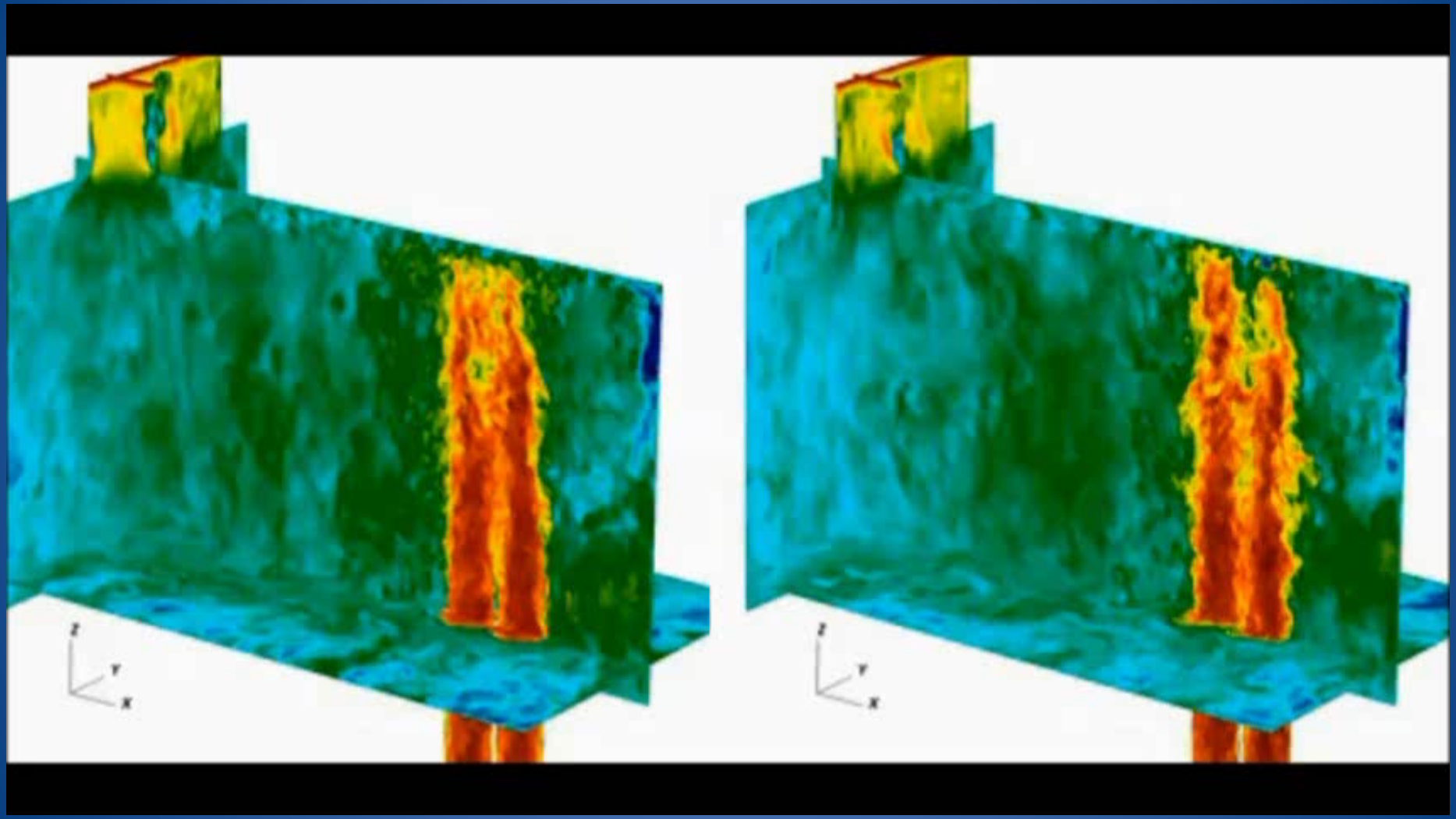
Scientists create and communicate
knowledge

Bambi on fire

Westworld

In flames

Computational Fluid Dynamics (CFD) simulations



A. Obabko, E. Merzari *et al*.

Computers enhance our brain;
they help us optimize and design

But is this real?

Model validation

Validation of CFD simulations - MAX facility

S. Lomperski *et al.*

The “Uncanny Valley”

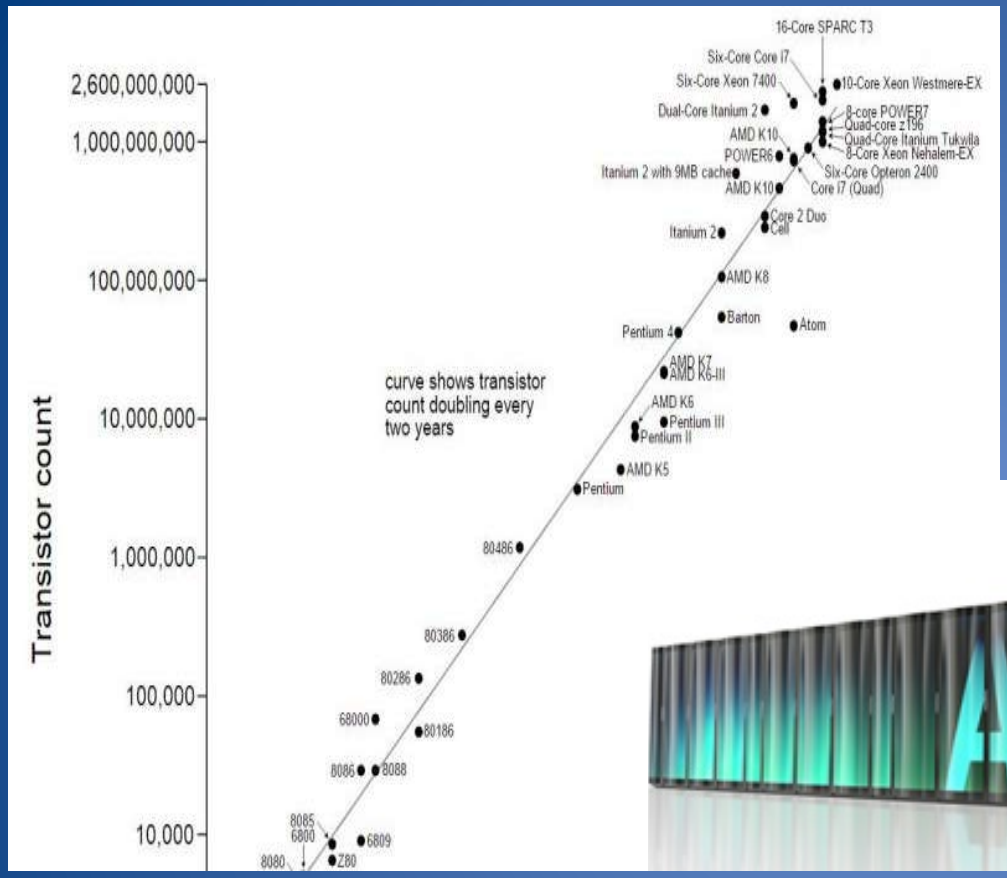
By Jorje Rivas, Discovery News

Predictions

You can't connect the dots looking forward; you can only connect them looking backward. So you have to trust that the dots will somehow connect in your future. ...
This approach has never let me down, and it has made all the difference in my life.

Steve Jobs

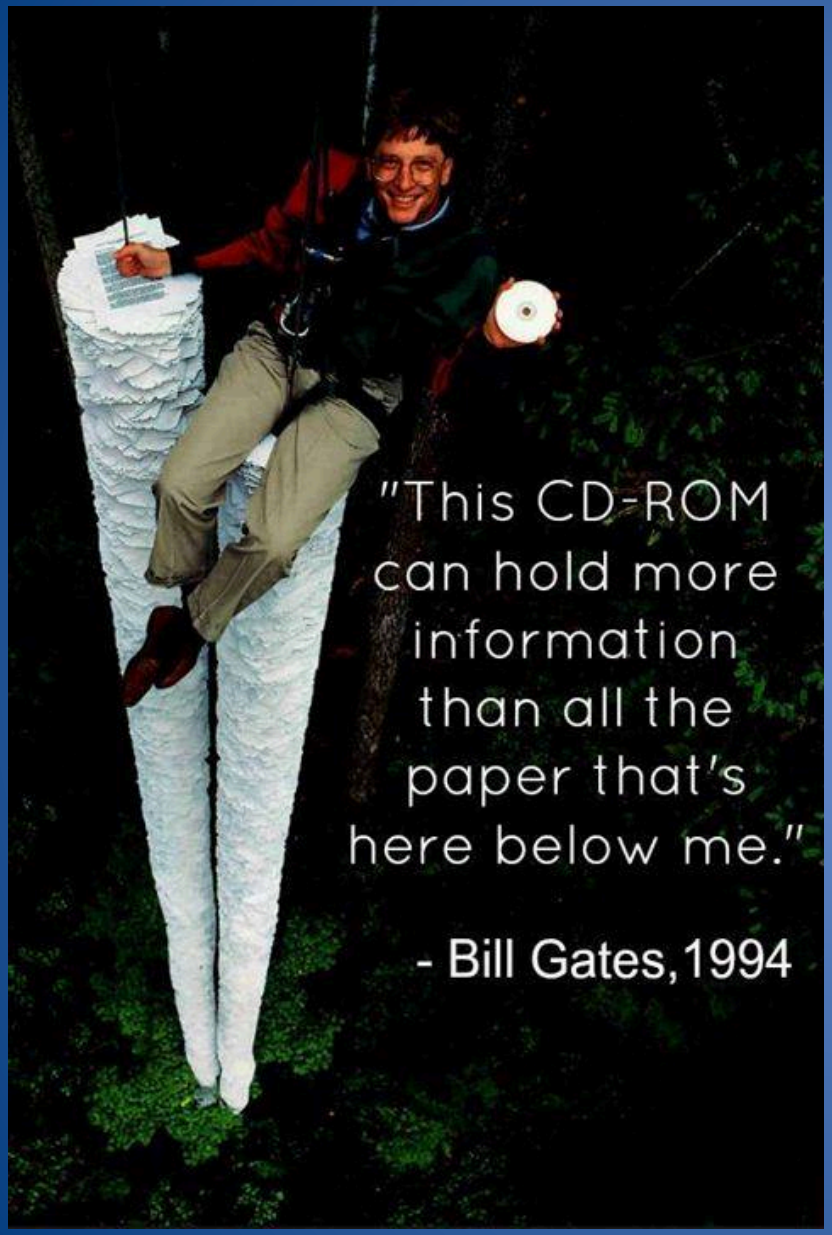
Moore's law and paper



"The future of integrated electronics is the future of electronics itself. The advantages of integration will bring about a proliferation of electronics, pushing this science into many new areas. Integrated circuits will lead to such wonders as home computers–or at least terminals connected to a central computer–automatic controls for automobiles, and personal portable communications equipment. The electronic wristwatch needs only a display to be feasible today."

G. Moore, Electronics, 38 (1965)

Memories

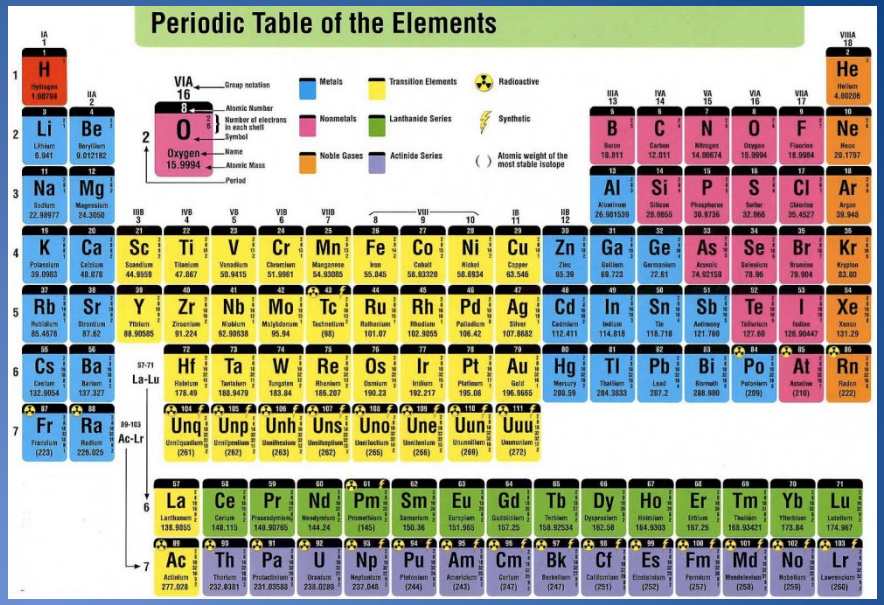


256GB USB Flash Drive
-SanDisk, 2015

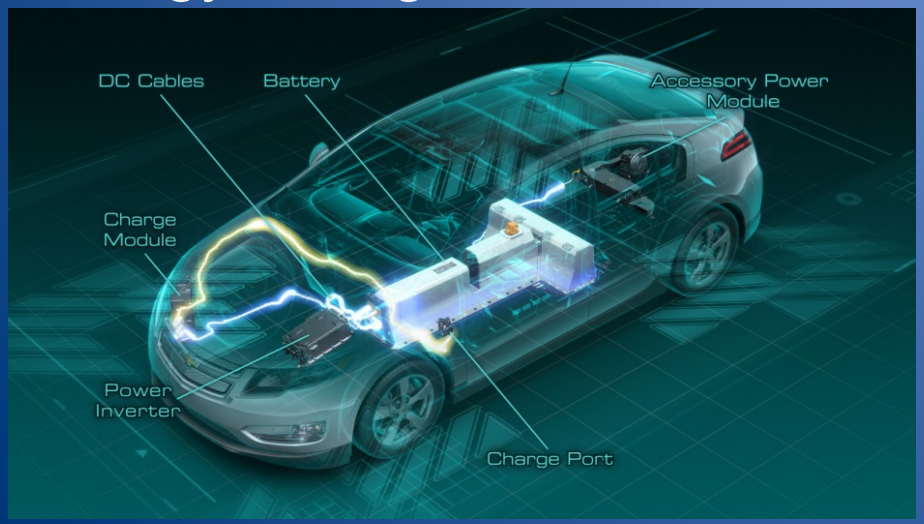
In the next 5 years

Energy production

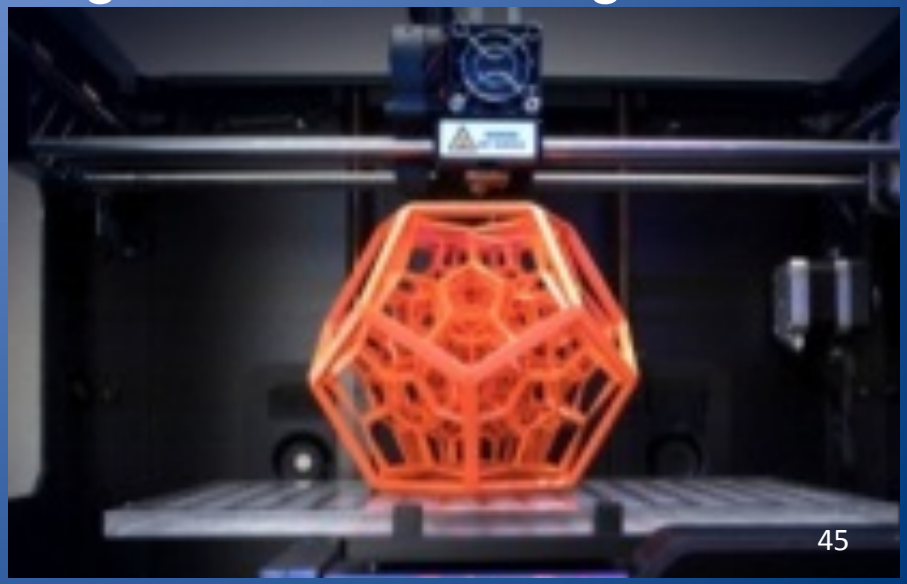
Materials Genome Initiative



Energy storage



Digital manufacturing



Final test

Predict the 2020 ranking of the top 5 programming models – by number of users.

Send to mstan@anl.gov by Aug. 31, 2015.

How to choose a profession

If you like to create something,
then be a scientist, engineer, actor, author, composer

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If you like to tell other people what to do,
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Whatever you do,
do it with all your heart!