ATPESC, St. Charles, Aug. 13, 2015

Computational Science and Cinema

Marius Stan







Breaking Bad



Sony Television Production ²

facebook Bogdan's Eyebrows

Blog entries:

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

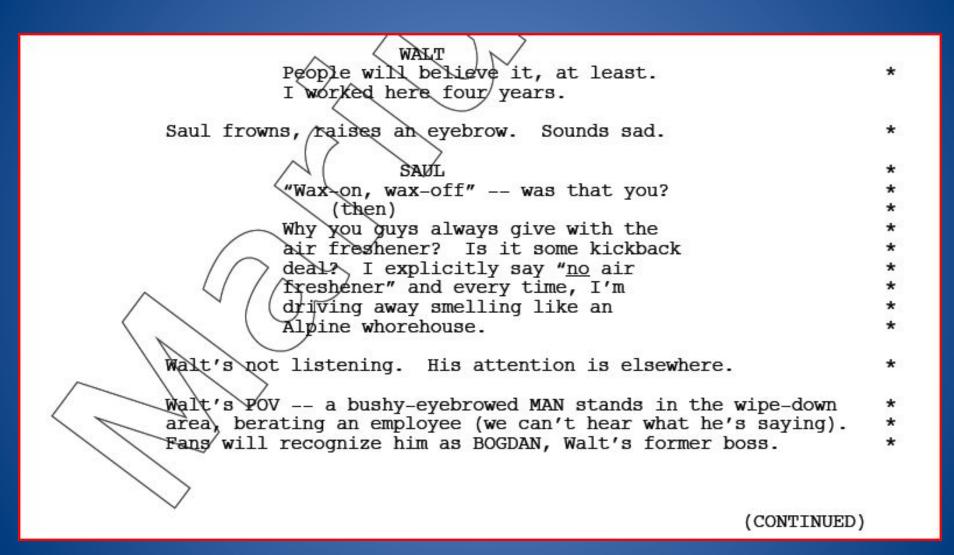
"He has a tumor."

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

"His mistress needs a new car."

A good script

Breaking Bad, Ep. 311, "Abiquiu"

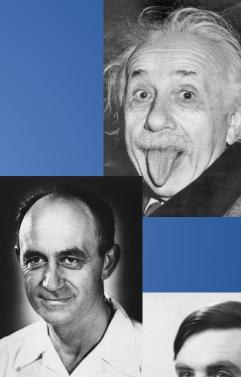


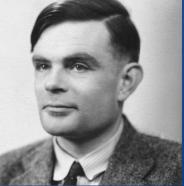
Breaking Bad, Ep. 311, "Abiquiu"

5

The Scientific Method

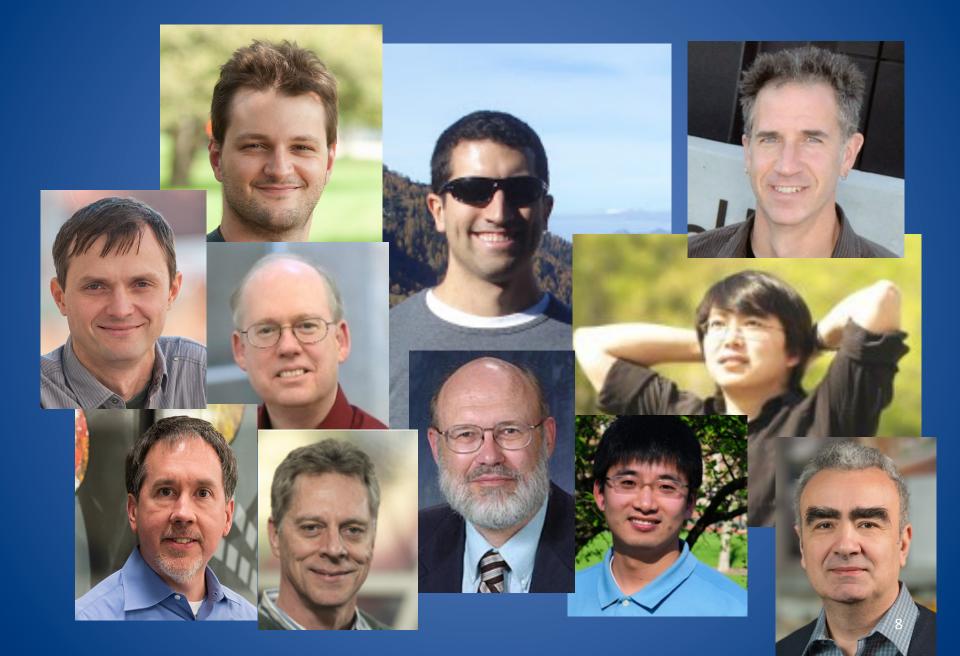
- Observation Question
- Hypothesis
- Model
- Prediction
- Validation
- Communication





A good team

Computational Scientists at Argonne







NUCLEAR ENERGY ADVANCED MODELING & SIMULATION PROGRAM

E. Merzari, A. Obabko et al.



Computation Institute University of Chicago M. Wild et al.



P. Voorhees, C. Wolverton et al.



Center for

G. Olson, O. Heinonen et al.



M. Welland, L. Curtiss et al.

At the Breaking Bad finale party in Hollywood, CA

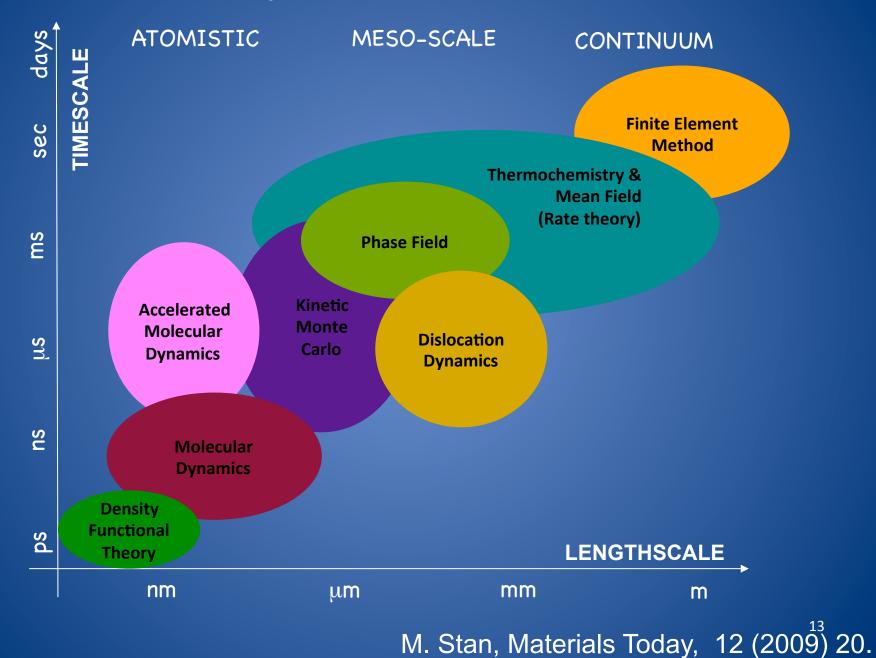




Quiet please.. Roll sound.. Roll Camera.. Action!



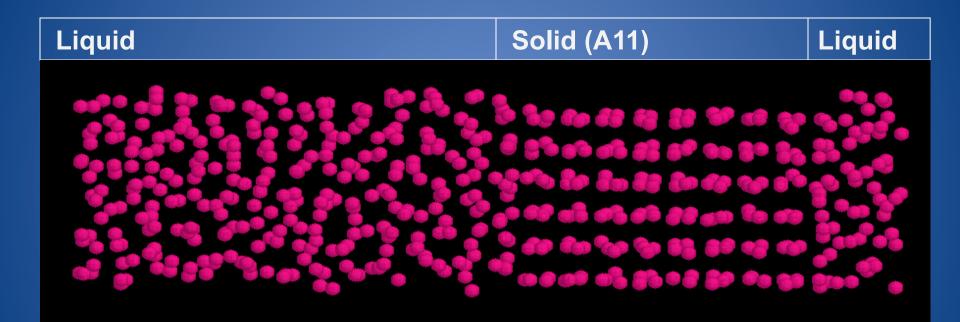
Multi-Physics and Multi-Scale



Melting of Gallium (Ga)



Melting – atom by atom



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 1	OTAL PAG	GES
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	518A 718A		a) 518A	
RJ MITTE	4k. WALTER JR.		H	HOLD HOLD		HO	OLD	
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	930A RPT @ 8		
	STAND-I	NS AND ATMO	SPHERE				SPECIALI	INSTR
SI (WALT - TIM)	RPT @ 7A					Please read the following safety memo-		
SI (JESSE / BODGAN - WILL) SI (SK YLER - VIKKI) SI (SAUL - ROBERT) SI (ANDREA - MONIQUE) SI (BROCK)	RPT @ 830A RPT @ 7A RPT @ 830A RPT @ 2P RPT @ 2P	1 BERATED EMPLOYEE RPT @ 615A Safety Memos for today: 32, 10 CAR WASH PATRONS W/ CARS 10 CAR WASH PATRONS W/ CARS RPT @ 630A (CARS WILL BE USED AT CAR WASH AS WELL AS TACO SAL'S) 2 COOKS RPT @ 2P						
Contraction of the Ann	AARA MATTERSON	2 WAITRESSES RPT @ 2P			5 (F 1 +)	BREAKFAST AND L		
PHOTO DBL. BROCK	RPT @ 1230P		L DINERS W/ CA		7421.0227	BRKFST	25/115	RE
		(CARS WILL	BE USED AT TAC	O SAL'S AS WELLA	S CAR WASH)		140	RE
		A	DVANCE SHOO	OTING SCHEDU	LE	19-22-24		1.4
SET DESCRIPT	SCENES		CAST	D/N	PGS		1.00	
	DAY 5	TUESDAY, DEC.	EMBER 15, 2009					
EXT - URBAN STREET		33	2, 25,	2, 25, 26, 27K., Atmos. D6		1 7/8 2ND & HA2		

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



Twenty million dollars!!!



Breaking Bad, Ep. 402, "Thirty-Eight Snub"

Twenty million gigaflops!!!





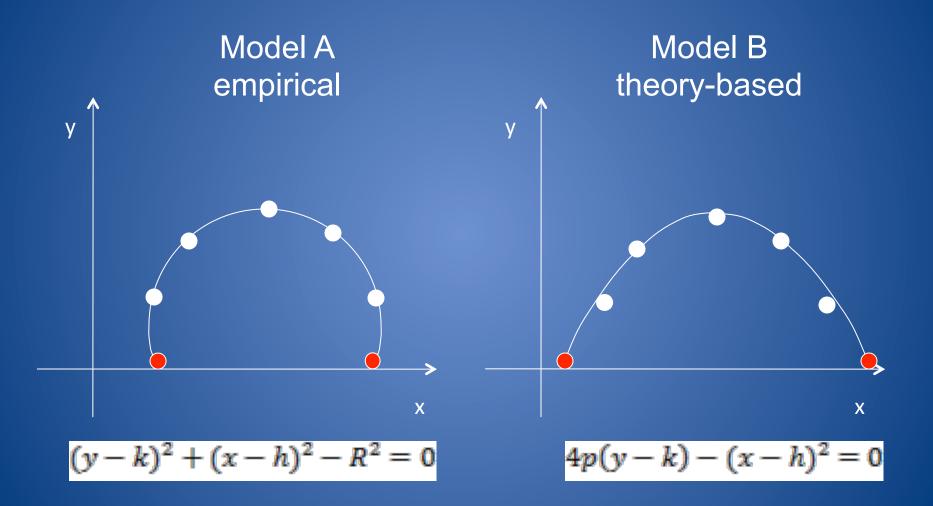
Argonne Leadership Computing Facility 24

Mid-term test

Object in a gravitational field - observation



Object in a gravitational field - predictions

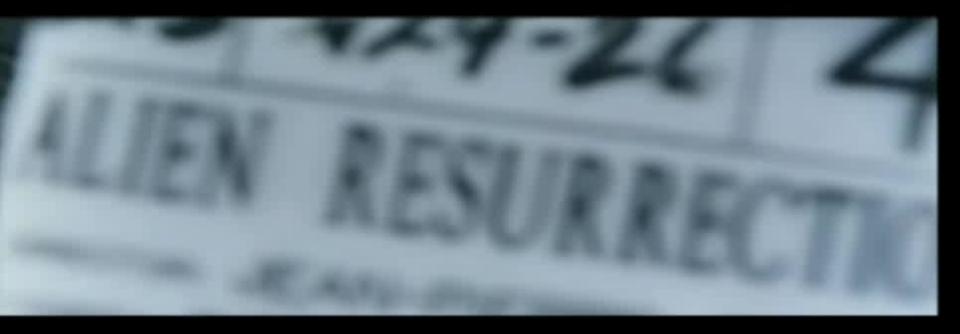


Theory-based models improve understanding and prediction

But is this correct?

Solution verification

Precision and accuracy



Alien Resurrection, 1997



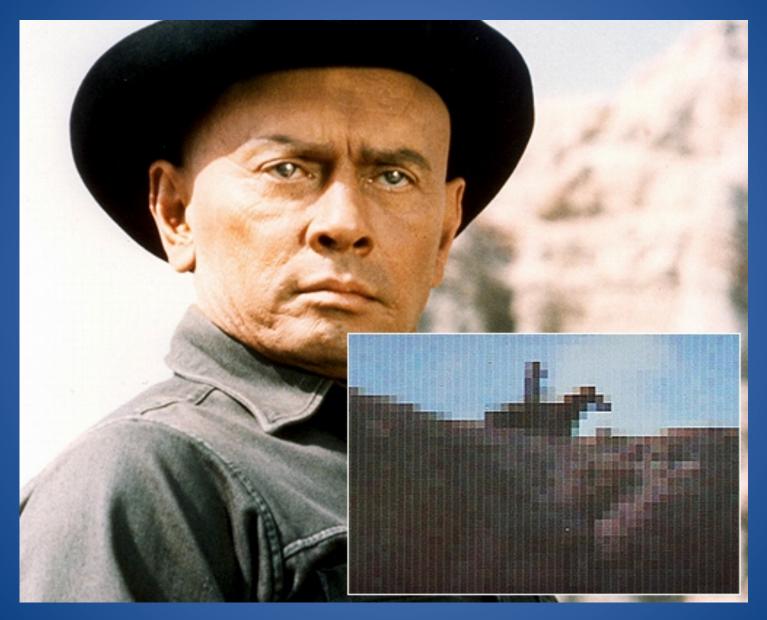
Artists create and communicate emotions

Scientists create and communicate knowledge

Bambi on fire



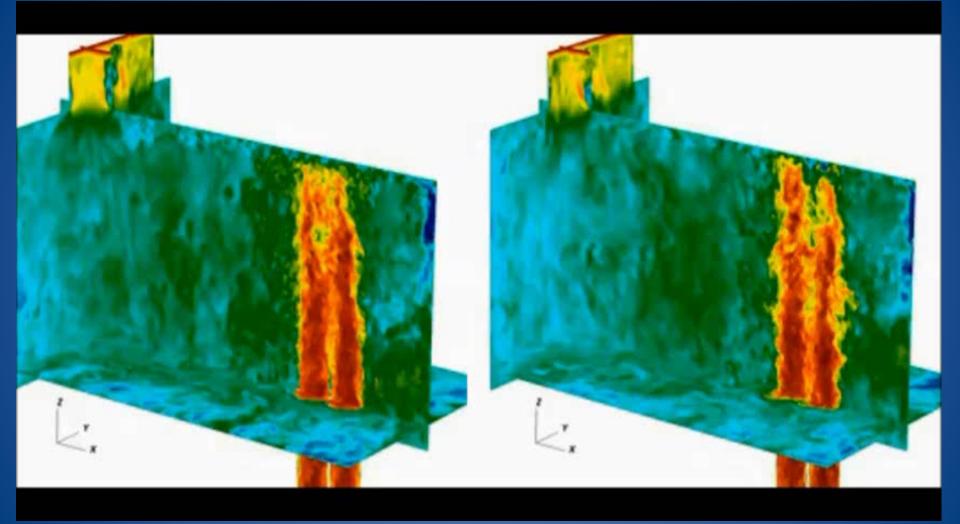
Westworld



In flames



Computational Fluid Dynamics (CFD) simulations



A. Obabko, E. Merzari *et a*l. ³⁶

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. 39

The "Uncanny Valley"



By Jorje Rivas, Discovery News

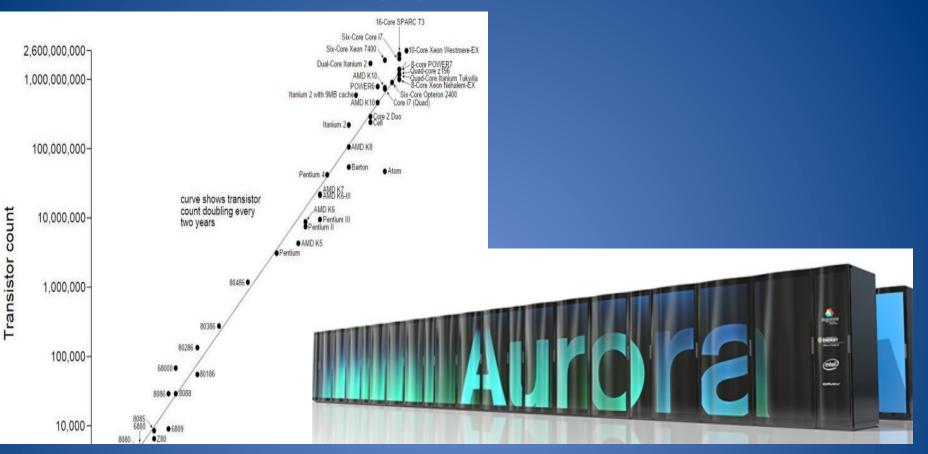
40

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

"This CD-ROM can hold more information than all the paper that's here below me."

- Bill Gates, 1994



256GB USB Flash Drive -SanDisk, 2015

In the next 5 years

Energy production

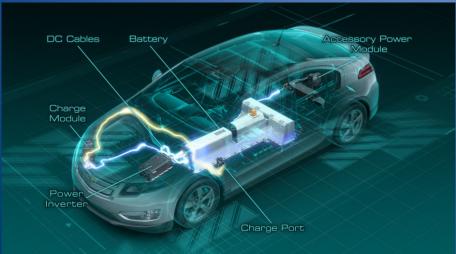


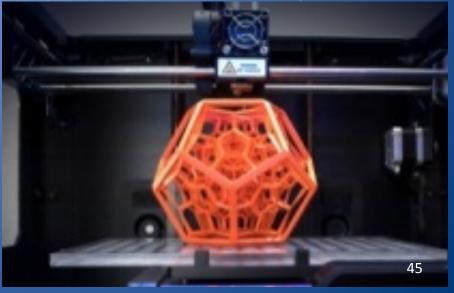
Materials Genome Initiative

Periodic Table of the Elements															18			
1	H Hytrogen 1:00784	IIA 2		VIA Group notation				Tr	ansition Eleme	nts 🔥	Radioactive		IIIA 13	IVA 14	VA 15	VIA 15	VIIA 17	2 He ² Hellen 4.00206
2	3 Li Lithiam 6.941	Beryfliam 9.012182	2 1	0, 0xygen+ 15.9994	Number of in each sh Symbol Name	electrons ell	Nonmeta Noble Ga		inthanide Serie ctinide Series	n 🦸	Synthetic Atomic weight of the most stable isotope			Carbon 12.011	Nitrogen 14.00674	0 ² Oxygen 15.9994	Flacrice 18.9984	Ne ² Neos 20.1797
3	Na 3 Sediam 22.98977	Magnesium 24.3050	IIIB 3	IVB 4	Period VB 5	VIB 6	VIIB 7	8		10	18 11	11B 12	13 Al ² Aluminum 26.981539	Silicon 28.0855	Phospharus 30.9736	18 Seitur 32.066	Chioritee 35.4527	18 Argon 39.948
4	Potassium 39.0983	Calcium 48.678	Scandium 44.9559	Titanium 47.867	28 V Vanadium 50.9415	Cr Cheomium 51.9961	Manganese 54.93085	kon 55.845	Cobalt 58.93328	28 Ni Hickel 58.6934	Copper 63.546	30 Zn 21nc 65.39	Ga Salliern 69.723	Germanium 72,61	AS 4 Acsenit 74.92159	Selesium 78.96	Br i Bramine 79.904	Krypten 83.80
5	Bebidium 85.4678	Strontium 87.62	39 Y Yttrium 88.90585	40 Zr Zirconiam 91.224	Nibium 92.90638	42 Molybdanam 95.94	Tcc IIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIII	Ratherium 101.07	45 Rh Phodiam 102.9055	Palladium 106.42	A7 Ag silver 107.8682	48 Cd Cadmiem 112,411	49 In 1 Indian 114.818	50 Sn Tie 118.718	SI Sb Autimony 121.760	Tellurium 127.60	53 I 126.90447	Xee 1 Xee 1 131.29
6	65 Cs Cestum 132.9054	Barlem 137.327	57-71 La-Lu	Hatataran 12 Hatataran 12 178.49	Tantalum 180.9479	74 W Tungsten 183.84	75 Re Rbenken 186.207	76 Osmium 190.23	17 17 17 11 11 11 11 11 11 11	Platinum 195.08	Au Geld 196.9665	Hg Mercury 200.59	81 TI 204.3853	82 Pb 1 Lead 207.2	83 Bismuth 208.980	Poloniam ¹⁴ (209)	Astaline 7 (210)	Rn in Raden in (222)
7	Francium 1	Radium 226.025	89-103 Ac-Lr	Unq	Unnipenius 2 (262)	Unh Unsilitation (263)	Uns	Uneilectium in (265)	Une united in the second secon	Ununsilier in (269)								
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Digital manufacturing

Energy storage







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

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

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

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If you like to serve society, then be a teacher, professor, doctor, soldier, lawyer

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> Whatever you do, do it with all your heart!