MEAM Interatomic Potential Generation: Coupling with MATLAB

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Collaborators: F. Gao[3], X. Sun[3], M. Khaleel[3]

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"On the topic of *Baskes-less* MEAM Interatomic Potential Development" **

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** PROCEEDINGS OF THE ROYAL SOCIETY A MATHEMATICAL, PHYSICAL & ENGINEERING SCIENCES

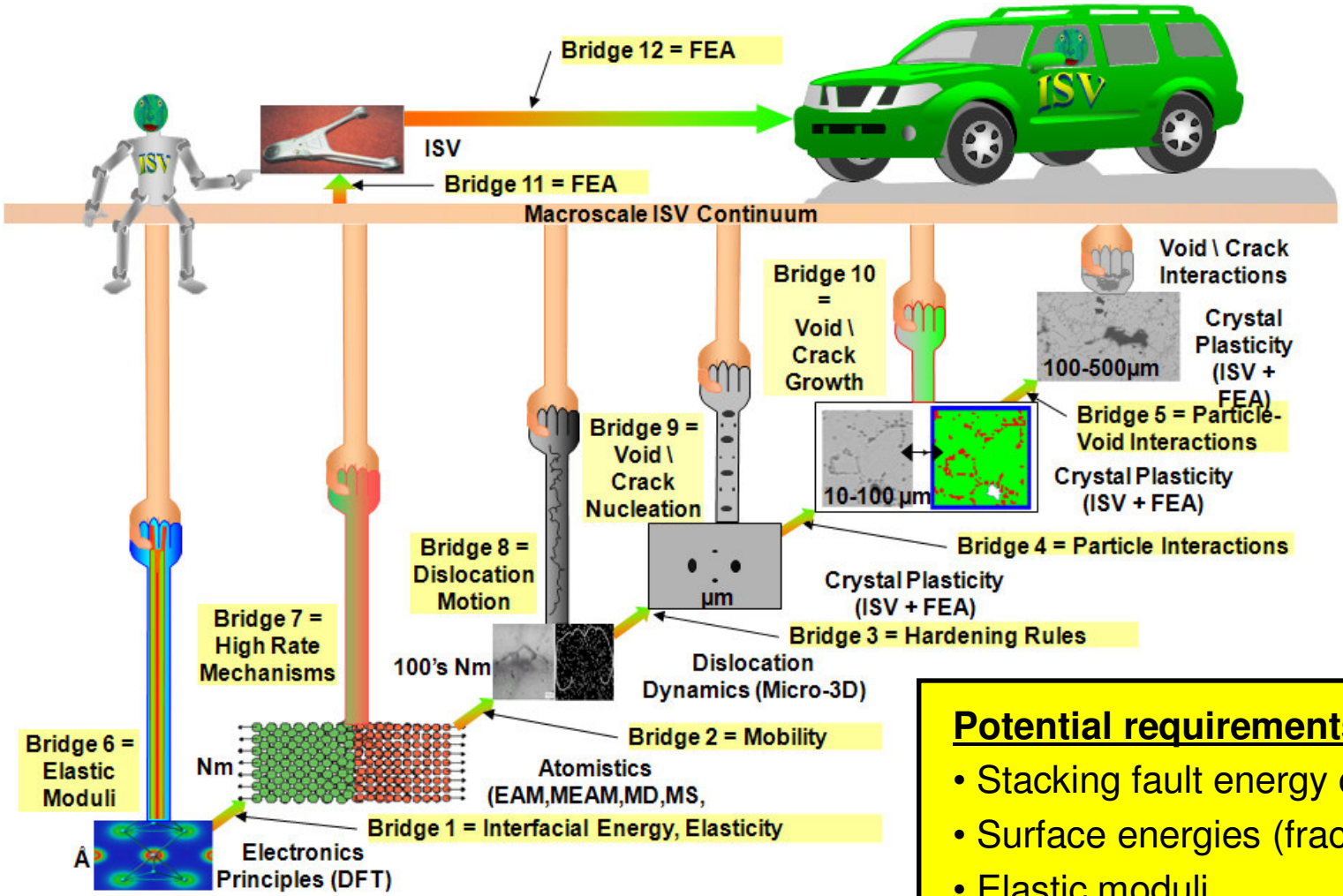
In preparation (2010) ☺

Outline

- Introduction
    - CAVS/Cyber-infrastructure/Motivation
- MATLAB Coupling with Atomistic Codes
- Fe-He MEAM Interatomic Potential
- Interatomic Potential Optimization Technique
- Monte Carlo Search
- Conclusions

Introduction

CAVS: Multiscale Models of Mechanical Behavior



Potential requirements

- Stacking fault energy curves
- Surface energies (fracture)
- Elastic moduli

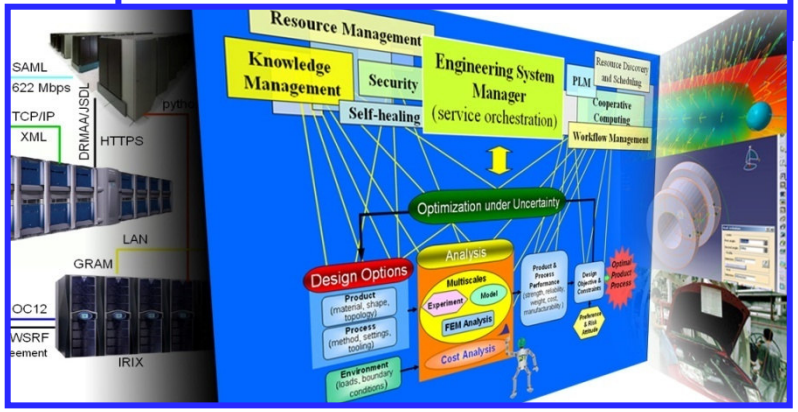
Introduction

***CAVS**: Cyberinfrastructure*

IT technologies
(hidden from the engineer)

Conceptual design process
(user-friendly interfaces)

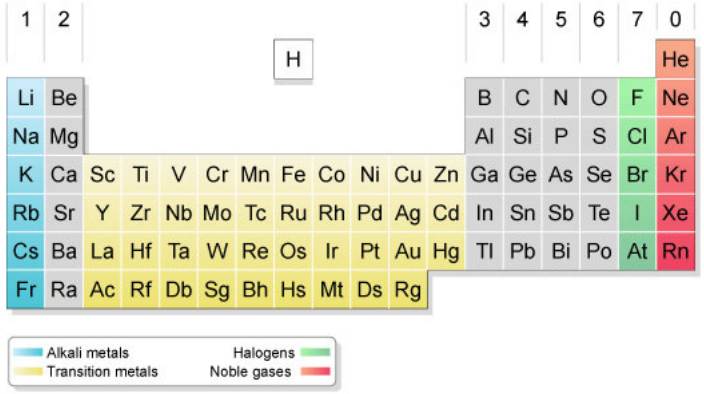
Engineering tools
(CAD, CAE, etc.)



ccg.hpc.msstate.edu

CAVS - MEAM Interatomic Potential Development

- Aluminum
  - Al-Mg, Al-Si, Al-Cu, Al-Fe, etc.
- Magnesium
  - Mg-Al, etc.
- Steel
  - Fe-V, Fe-C, etc.



- Nuclear Applications
- Polymer/composites

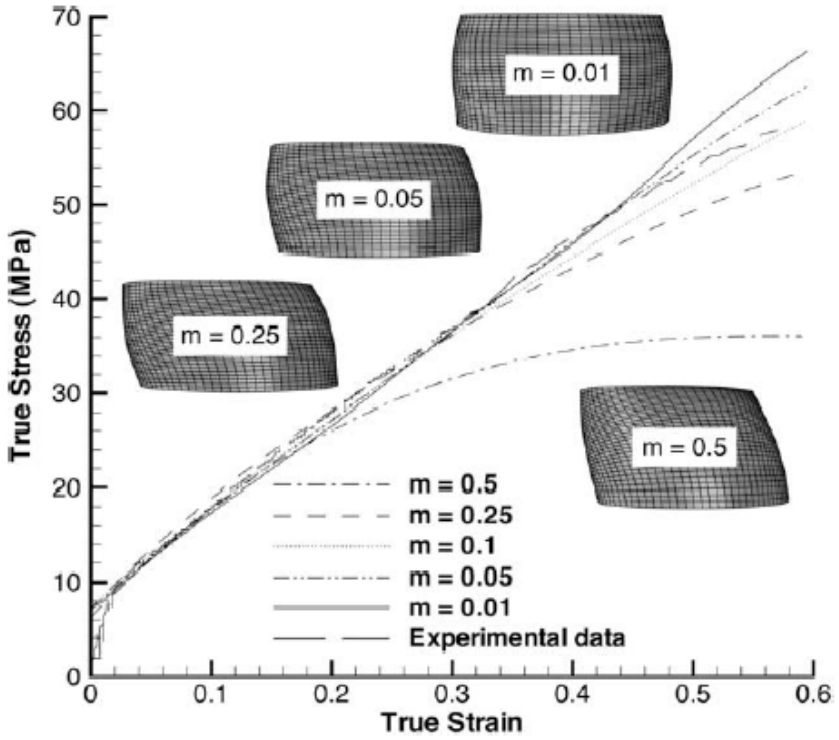
New research areas

Still needs some work…

- Needs to be efficient!!!
- Optimization techniques – what methodology works best?
- Ease of transferability to new potentials
- Addition of new response variables (e.g., stacking fault energy)

Dislocation mobilities for Al multiscale models

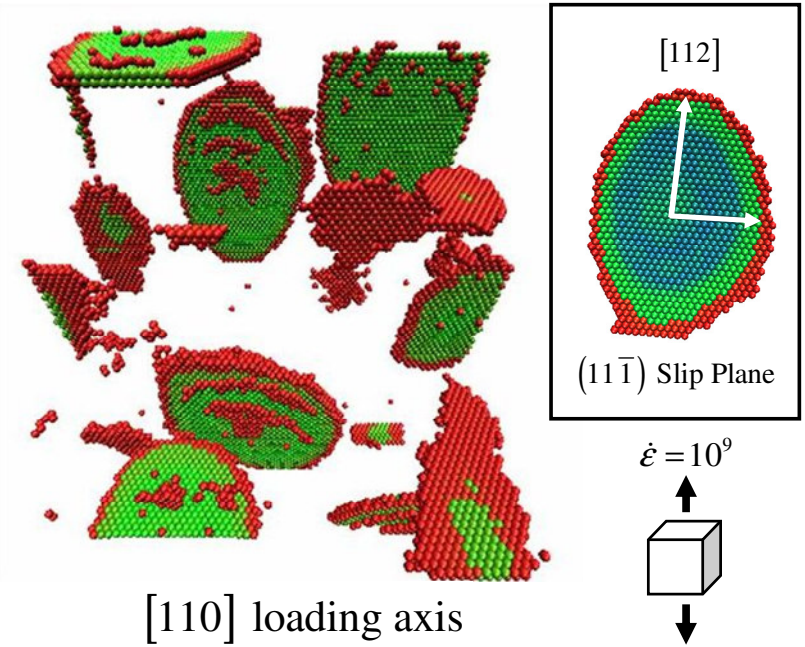
Groh, Marin, Horstemeyer, Zbib, IJP (2009)



Introduction

Dislocation mobilities for Al multiscale models

Single crystal dislocation nucleation
Tschopp, McDowell, JMPS (2009)

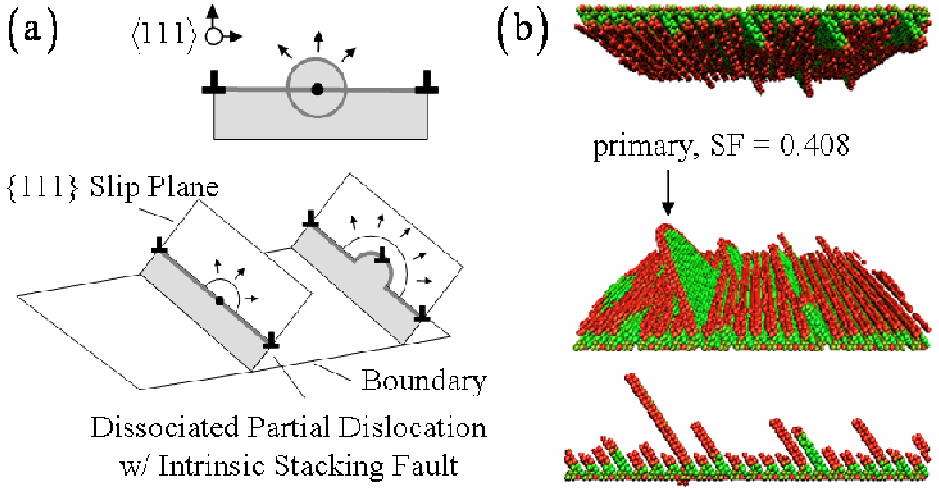


Introduction

Dislocation mobilities for Al multiscale models

Single crystal dislocation nucleation

Grain boundary dislocation nucleation
Tschopp, McDowell, IJP (2008)



Introduction

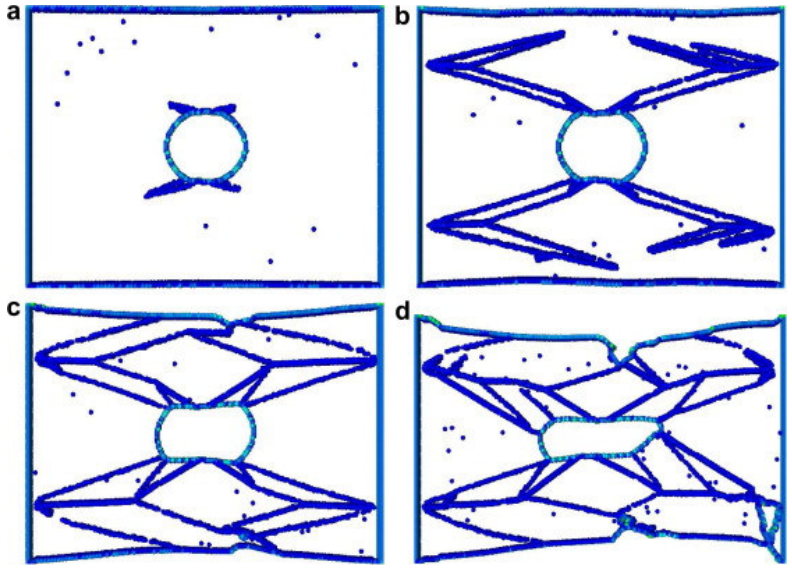
Dislocation mobilities for Al multiscale models

Single crystal dislocation nucleation

Grain boundary dislocation nucleation

Void growth and coalescence

Tang, Kim, Horstemeyer, Acta Materialia (2010)



Introduction

Dislocation mobilities for Al multiscale models

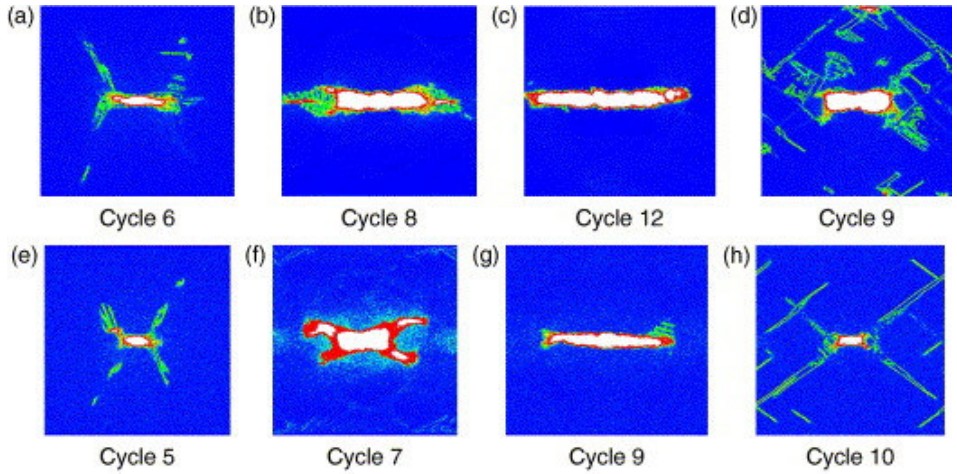
Single crystal dislocation nucleation

Grain boundary dislocation nucleation

Void growth and coalescence

Fatigue and Damage

Potirniche, Horstemeyer, et al. IJF (2005)



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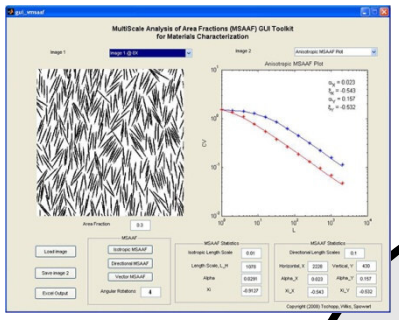
MATLAB Coupling w/ External Atomistic Codes

Introduction

Tschopp et al. MSMSE (2009),
Wilks et al. MSEA (2010)

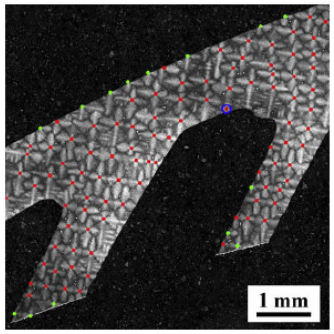


Spline Fitting

Genetic Algorithm

Neural Network

Image Processing →



Tschopp et al. ScrMater (2010)

Optimization

Parallel Processing

Toolboxes

GUI

MATLAB

External Programs

Data Management

DYNAMO

VASP

LaTex

LAMMPS

GNUPLOT

ABAQUS

VPSC

***.mat datafiles**

Write to Excel

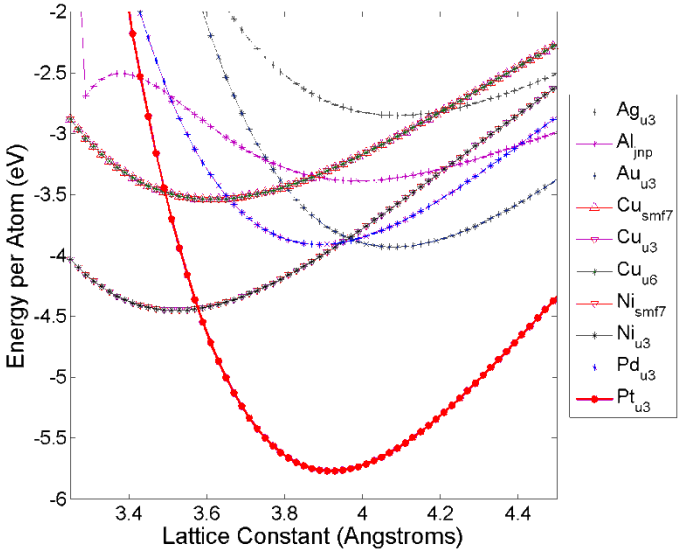
Output images

Generate LaTex reports

Write to *.ppt

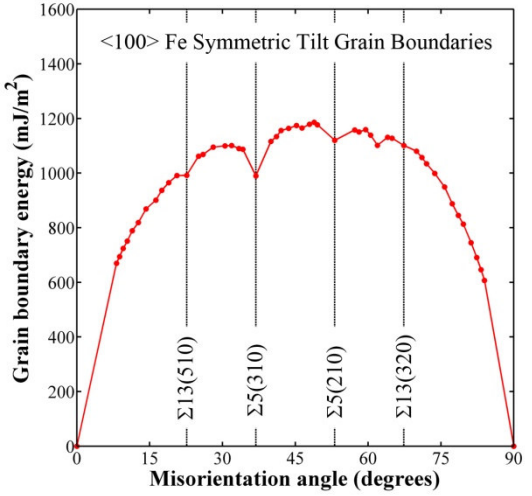
***.fig graphs**

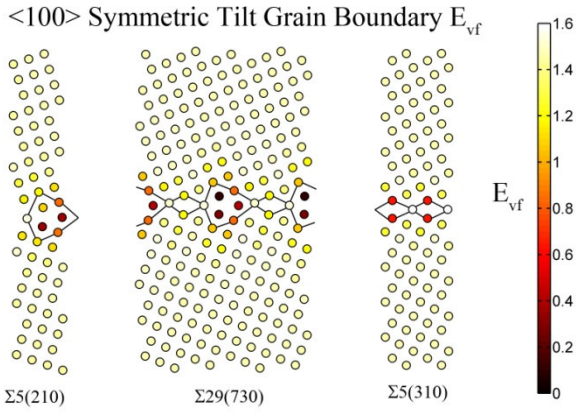
How do we generate the energy per atom for 10 different EAM potentials as a function of lattice constant? How do we do it quickly?



MATLAB coupled with LAMMPS Windows executable

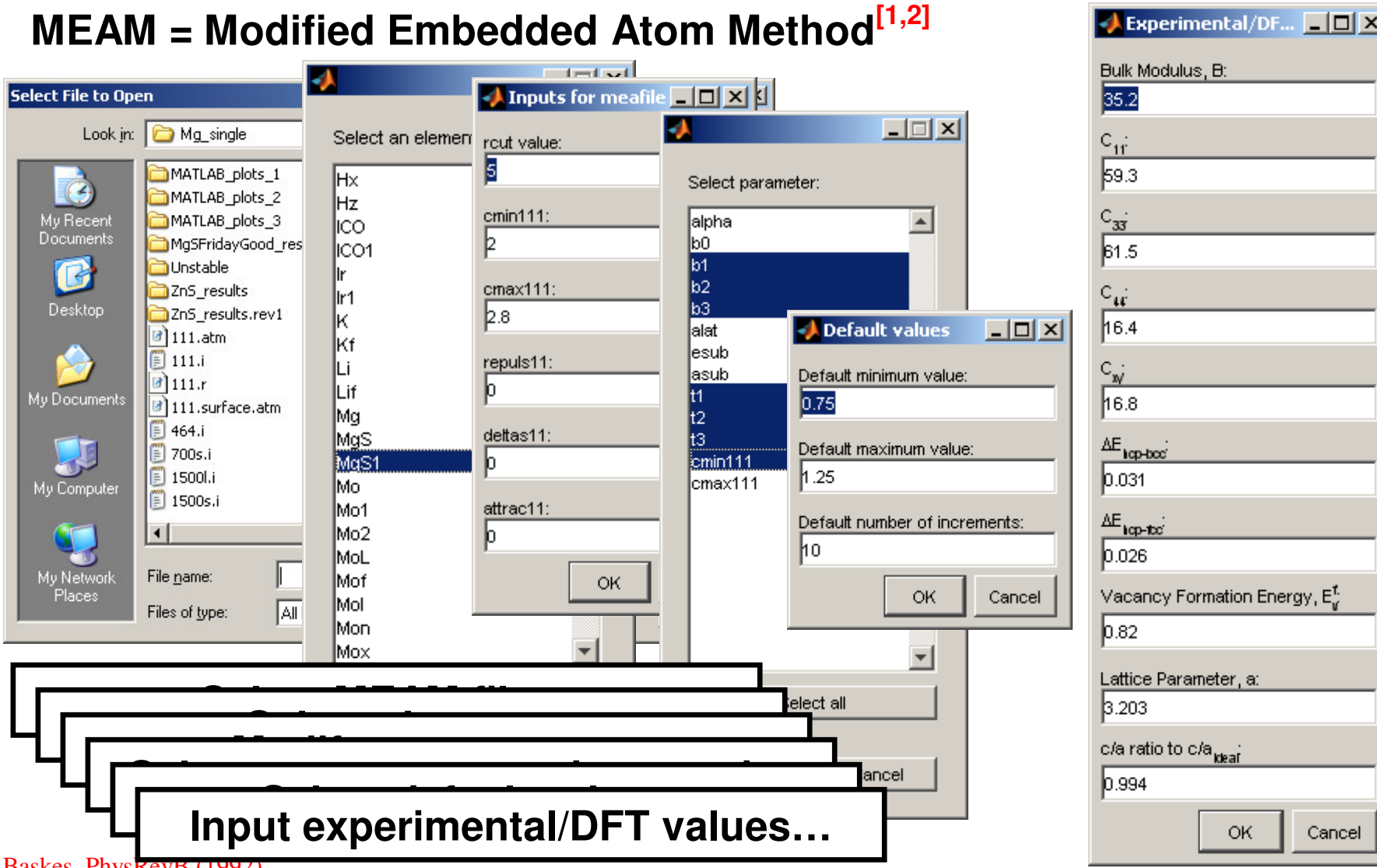
(~70 sec for 250 simulations)





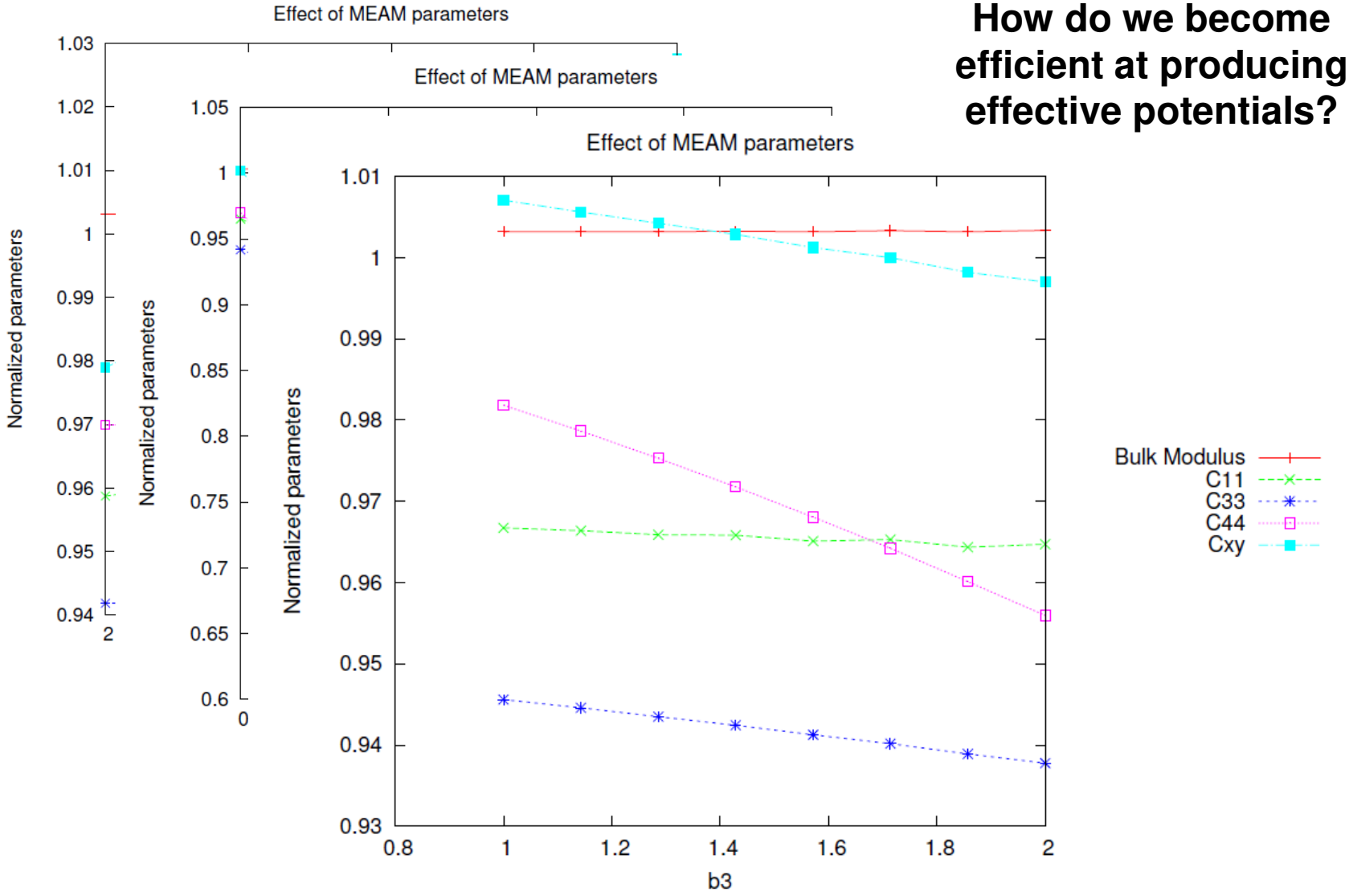
MEAM Interatomic Potential Development
One-At-a-Time Optimization

MEAM = Modified Embedded Atom Method[1,2]



[1] Baskes, PhysRevB (1992)
[2] Baskes, Johnson, MSMSE (1994)

MEAM Interatomic Potential Development
One-At-a-Time Optimization



How do we become efficient at producing effective potentials?

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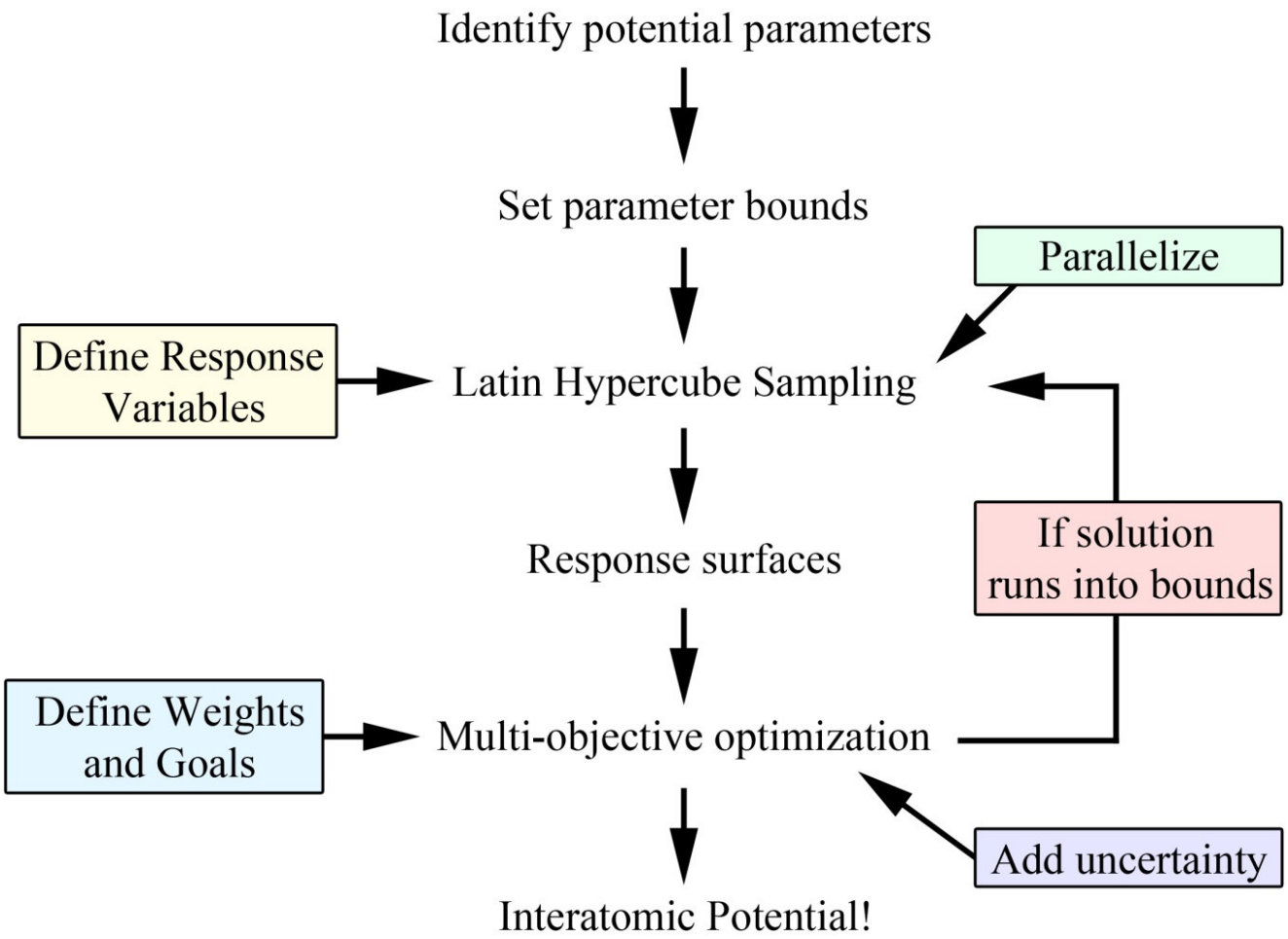
MEAM Interatomic Potential Development Optimization Technique: Application to Fe-He

MEAM Interatomic Potential Development Methodology



MEAM Interatomic Potential Development
Fe-He parameters

Single element MEAM parameters

Parameter	Fe	He
alpha	5.027	8.350
alat	2.851	4.100
esub	4.280	0.032
asub	0.555	1
attrac/repuls11	0.150	0
rozero	1	0.450
Cmin111	0.8	2.0
Cmax111	1.9	2.8
b0	3.5	6.06
b1	2	6.06
b2	1	6.06
b3	1	6.06
t0	1	1
t1	-1.6	0
t2	12.5	0
t3	-1.4	0

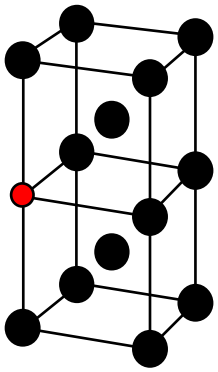
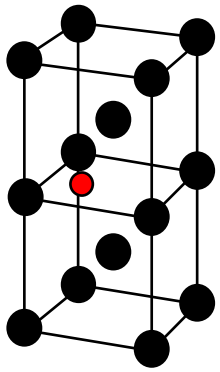
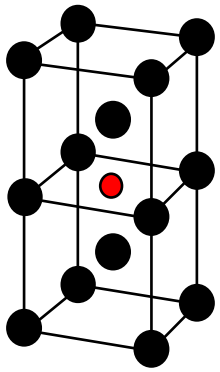
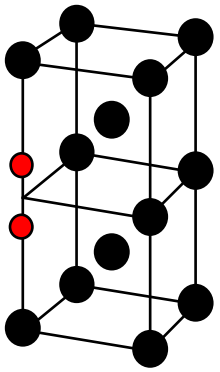
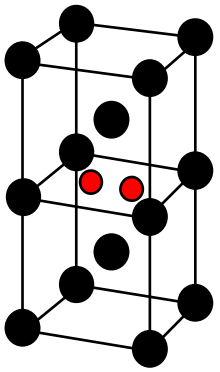
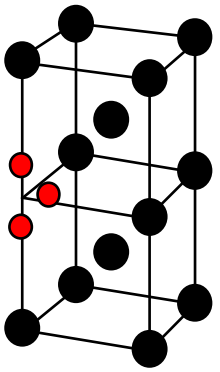
EAM

Fe-He interaction MEAM parameters

Parameter	Fe-He
rcut	4
rho2	0.34
alpha12	3.0
attrac/repuls12	0.10
delta12	1.14
Cmin112	2.0
Cmin121	2.0
Cmin122	2.0
Cmin211	2.0
Cmin212	2.0
Cmin221	2.0
Cmax112	2.8
Cmax121	2.8
Cmax122	2.8
Cmax211	2.8
Cmax212	2.8
Cmax221	2.8

MEAM Interatomic Potential Development
Fe-He parameters

Fe-He response variables

E_{sub}	$E_{tetrahedral}$	$E_{octahedral}$	E_{He_2V}	E_{He_2}	E_{He_3V}
4.00 eV	4.37 eV	4.60 eV	6.61 eV	8.79 eV	9.28 eV

Lowest energy in <100>

Didn't initially run…

Stoller, Selestkaia et al (ORNL)

MEAM Interatomic Potential Development
Fe-He parameters

INPUT

Single element MEAM parameters

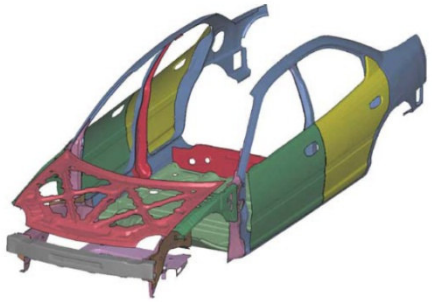
Parameter	Fe	He
alpha	5.027	8.350
alat	2.851	4.100
esub	4.280	0.032
asub	0.555	1
attrac/repuls11	0.150	0
rozero	1	0.450
Cmin111	0.8	2.0
Cmax111	1.9	2.8
b0	3.5	6.06
b1	2	6.06
b2	1	6.06
b3	1	6.06
t0	1	1
t1	-1.6	0
t2	12.5	0
t3	-1.4	0

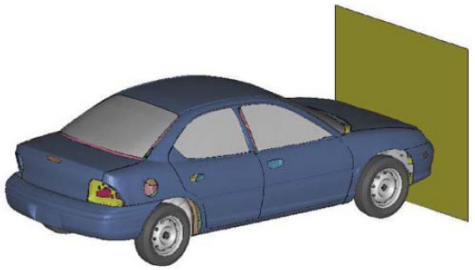
EAM

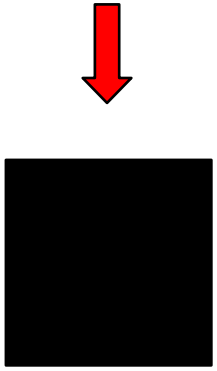
Fe-He interaction MEAM parameters

Parameter	Low	High
rcut	4	5
rho2	0.31	0.37
alpha12	2.7	3.3
attrac/repuls12	0.05	0.15
delta12	1.03	1.25
Cmin112	1.6	2.4
Cmin121	1.6	2.4
Cmin122	1.6	2.4
Cmin211	1.6	2.4
Cmin212	1.6	2.4
Cmin221	1.6	2.4
Cmax112	2.6	3
Cmax121	2.6	3
Cmax122	2.6	3
Cmax211	2.6	3
Cmax212	2.6	3
Cmax221	2.6	3

Can multiobjective crash optimization framework for side and roof impacts help?

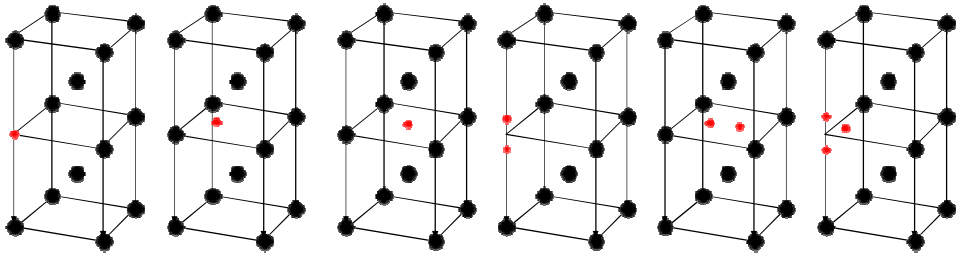






OUTPUT

Fe-He response variables



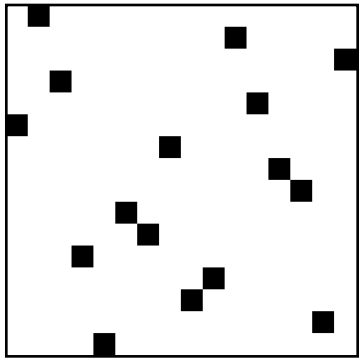
Acar, Solanki, *Struct Multidisc Optim* 39 (2009) 311.

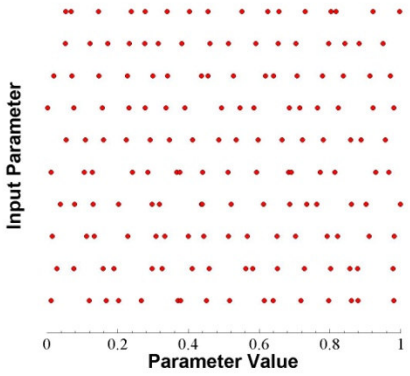
MEAM Interatomic Potential Development
Latin Hypercube Sampling

What is the most efficient way to sample n-dimensional parameter space?

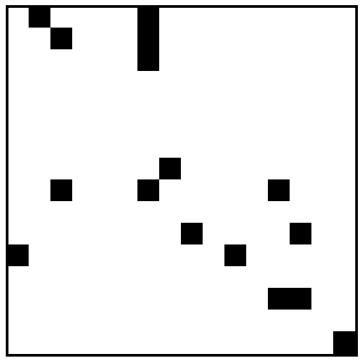
0 Parameter Space 1

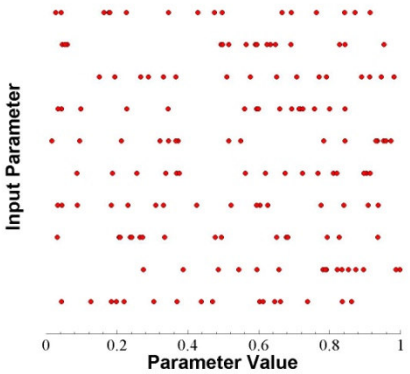
LHS design





Random sampling





- *Options - Reduce correlation or Maximize minimum distance*
- *Less evaluations needed!*

Now expand to *n*-dimensional space for each variable, generate LHS for x values of each variable (~2000+ here), and evaluate response variables

MEAM Interatomic Potential Development
Response Surface Fitting

Response Surface Methodology

$$f(x) = \beta_0 + \sum_{i=1}^{m} \beta_i x_i$$ linear

$$f(x) = \beta_0 + \sum_{i=1}^{m} \beta_i x_i + \sum_{i=1}^{m} \beta_{ii} x_i^2$$ quadratic

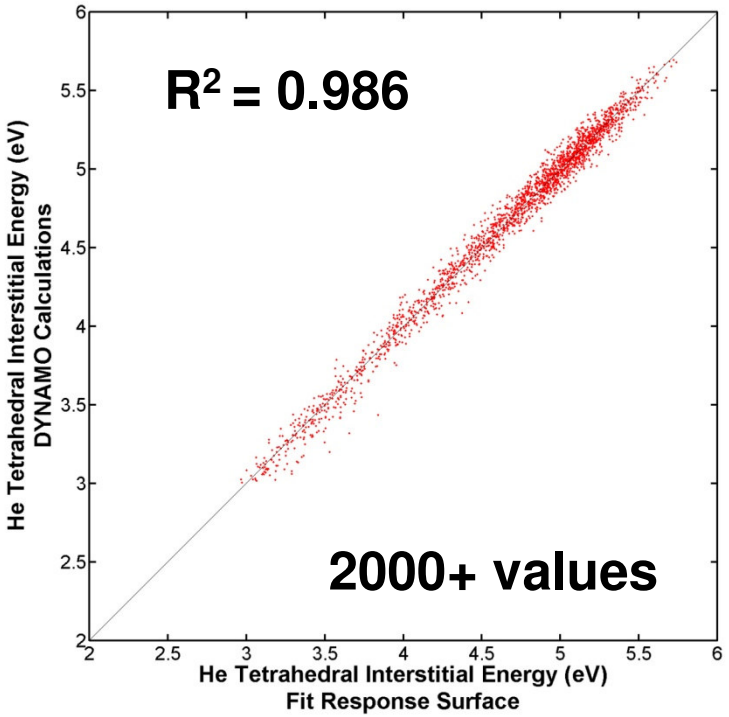
$$f(x) = \beta_0 + \sum_{i=1}^{m} \beta_i x_i + \sum_{i=1}^{m-1} \sum_{j=i+1}^{m} \beta_{ij} x_i x_j$$ interactions

$$f(x) = \beta_0 + \sum_{i=1}^{m} \beta_i x_i + \sum_{i=1}^{m} \beta_{ii} x_i^2 + \sum_{i=1}^{m-1} \sum_{j=i+1}^{m} \beta_{ij} x_i x_j$$ full quadratic

$$f(x) = \beta_0 + \sum_{i=1}^{m} \beta_i x_i + \sum_{i=1}^{m} \beta_{ii} x_i^2 + \sum_{i=1}^{m} \beta_{iii} x_i^3$$ cubic

$R^2 > 0.95$

He Tetrahedral Interstitial Energy



Response: 1 r2: 0.927, Response: 2 r2: 0.986
Response: 3 r2: 0.997, Response: 4 r2: 0.995
Response: 5 r2: 0.965, Response: 6 r2: 0.997

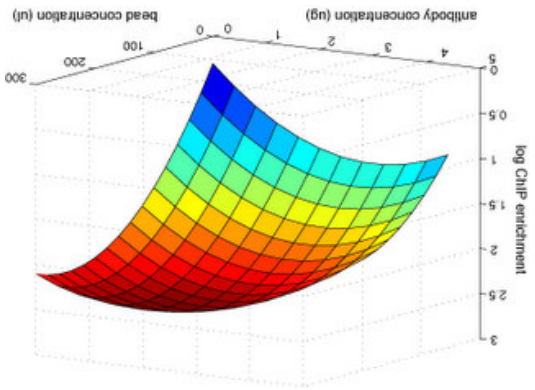
MEAM Interatomic Potential Development
Constrained Nonlinear Optimization

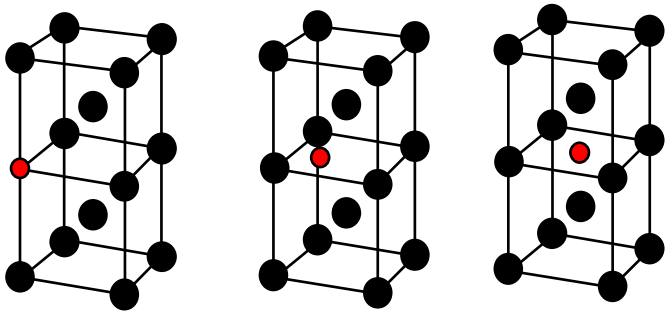
$$F(x) = \sum_{i=1}^{p} W_i \left(f_i(x) - g_i(x) \right)^2$$

$$Min\ F(x), \text{such that}$$

$$x_k^{lower} \le x_k \le x_k^{upper} \text{ for } k = 1, NDV$$

$$\sum_{i=1}^{p} W_i = 1,\ W_i > 0$$

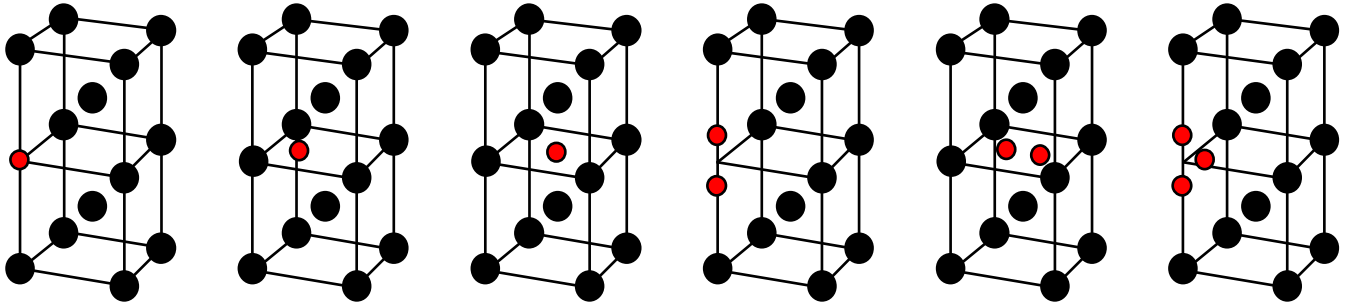




	E_{sub}(eV)	E_{tetra}(eV)	E_{octa}(eV)
W_i	1/3	1/3	1/3
VASP	4.00	4.37	4.60
RSM	4.00	4.37	4.60
DYNAMO	3.96	4.43	4.61

Success? …

MEAM Interatomic Potential Development
Fe-He parameters



	E_{sub}(eV)	E_{tetra}(eV)	E_{octa}(eV)	E_{He2V}(eV)	E_{He2}(eV)	E_{He3V}(eV)
W_i	1/6	1/6	1/6	1/6	1/6	1/6
VASP	4.00	4.37	4.60	6.61	8.79	9.28
RSM	4.00	4.37	4.60	6.61	8.79	9.28
DYNAMO	4.00	4.43	4.63	7.31	8.37	8.47

Ran for 100+ starting points, always biased similarly!

Advantage of doing optimization on response surface!!!

R^2>0.96, but metamodel isn't accurately capturing DYNAMO response

MEAM Interatomic Potential Development
Monte Carlo (Random) Search…

16,500 potentials sampled

$$E_{\mathrm{He_2V,<100>}} < E_{\mathrm{He_2V,<110>}}$$

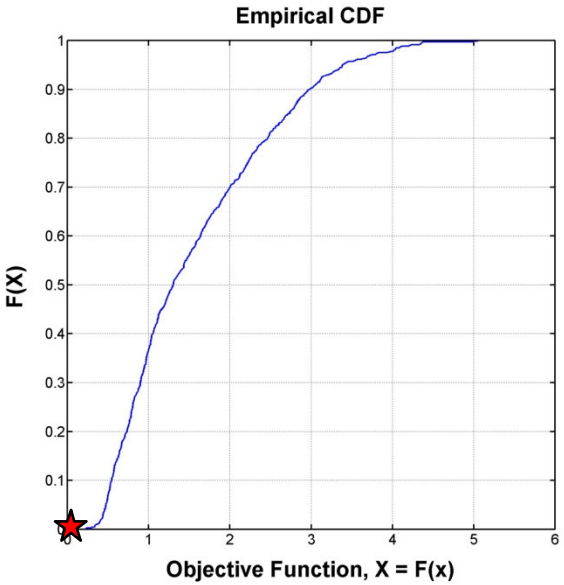
$$E_{\mathrm{He_2V,<100>}} < E_{\mathrm{He_2V,<111>}}$$

$$E_{\mathrm{He_2}} > 8 \text{ eV}$$

$$E_{\mathrm{He_3V}} > 8 \text{ eV}$$

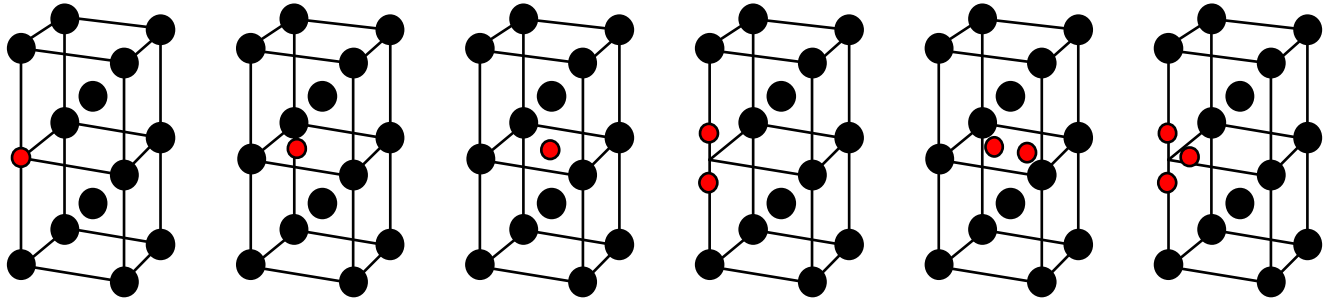
729 potentials

$$F(x) = \sum_{i=1}^{p} W_i \left(f_i(x) - g_i(x) \right)^2$$



What is the best potential based on these goals and constraints?

MEAM Interatomic Potential Development
Fe-He parameters



	E_{sub}(eV)	E_{tetra}(eV)	E_{octa}(eV)	E_{He2V}(eV)	E_{He2}(eV)	E_{He3V}(eV)
W_i	1/6	1/6	1/6	1/6	1/6	1/6
VASP	4.00	4.37	4.60	6.61	8.79	9.28
DYNAMO	4.00	4.63	4.83	6.32	8.65	9.48

Iterative refinement of bounds…?

Feed into simplex optimization technique now…?

Summary

- MATLAB can be a powerful tool for coupling atomistic codes with optimization methods for interatomic potential development
- How do we optimize interatomic potentials efficiently?
  - Parameter screening – which parameters are important for response surfaces?
  - What are the appropriate metamodels for each response variable?

Questions/Discussion?