

MEAM Interatomic Potential Generation: Coupling with MATLAB

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

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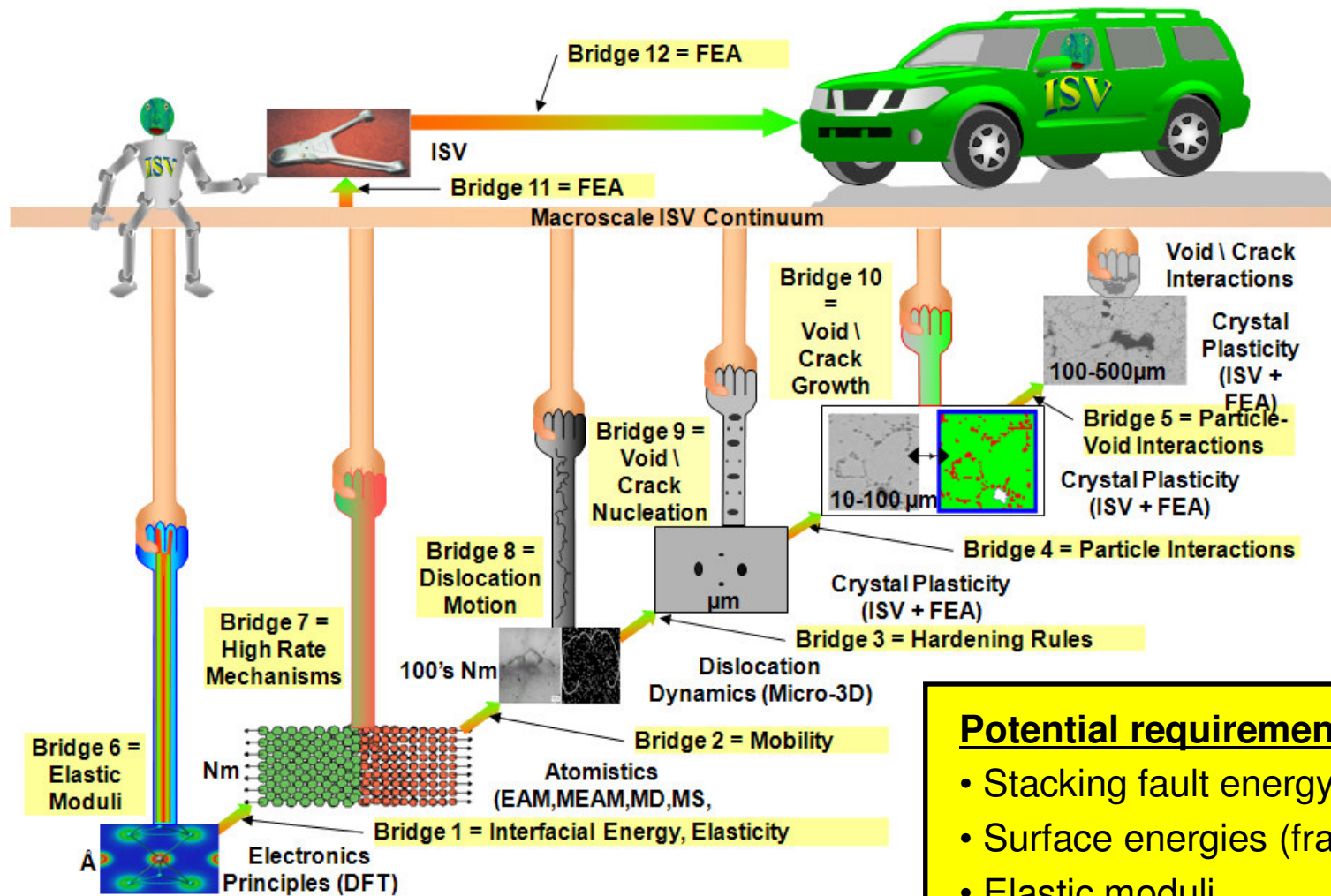
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³Pacific Northwest National Laboratory

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

CAVS: Multiscale Models of Mechanical Behavior



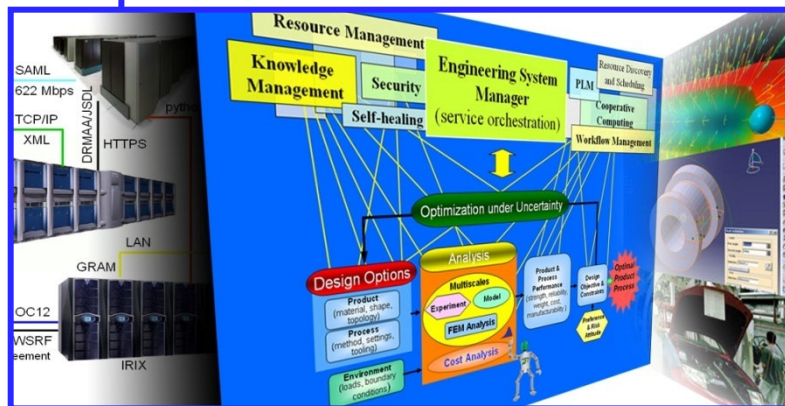
- Potential requirements**
- Stacking fault energy curves
 - Surface energies (fracture)
 - Elastic moduli

CAVS: Cyberinfrastructure

IT technologies
(hidden from the engineer)

Conceptual design process
(user-friendly interfaces)

Engineering tools
(CAD, CAE, etc.)



ccg.hpc.msstate.edu

Engineering Virtual Organization for CyberDesign

USAMP's Integrated Computational Material Engineering (ICME) and Southern Regional Center for Innovative Lightweight Design (SRCLID) supported by the Department of Energy (DOE)

Welcome!

Welcome to our Materials CyberSpace! Included in this CyberSpace is a collection of materials databases and multiple size scale codes so that one can design and develop the next generation materials and structural components. Our hope is that the creation of this cyberinfrastructure will result in the development of the "community of practice" portal that allows development and integration of multiscale physics-based materials models for selected properties and processes, in the context of United States Automotive Materials Partnership (USAMP) three-nation Magnesium Front-End Research and Development pilot project (MFERD) in particular task 1.9: Cyberinfrastructure for Integrated Computational Material Engineering (ICME).

There are separate web sites that provide more information on the MFERD and ICME projects. If you have any questions or comments regarding this website, please feel free to contact us at haupt@cavs.msstate.edu. Thanks and have fun light weighting your designs using our tools.

Sincerely,
Dr. Tomasz Haupt, CAVS Professor at Mississippi State University (MSU)
Dr. Mark Horstemeyer, CAVS Chair Professor at Mississippi State University (MSU)

This effort is funded by the Center for Advanced Vehicular Systems (CAVS) at MSU, the U.S. Department of Energy under contract 4000054701, and the NSF grant Virtual Organization for CyberDesign (Award ID: 0742730).

Call for Participation

The Cyberinfrastructure team created the infrastructure for web-based collaborative efforts. The success of this effort critically depends on the participation of the community towards the generation of the contents that will aid the research in Materials Science and lightweight innovative design. The expected community contributions are:

- Creating and updating pages in this Wiki. Please, refer to [Help with Wiki](#) tutorial on how to create and edit Wiki pages.
- Experimental data, material models, material constants, and codes at any length scale. Please refer to help sections available from [services](#) toolbox.
- Specifications for the requirements of the Cyberinfrastructure by adding to the [projects](#) pages.

Material Models at different length scales

Click on image to enter

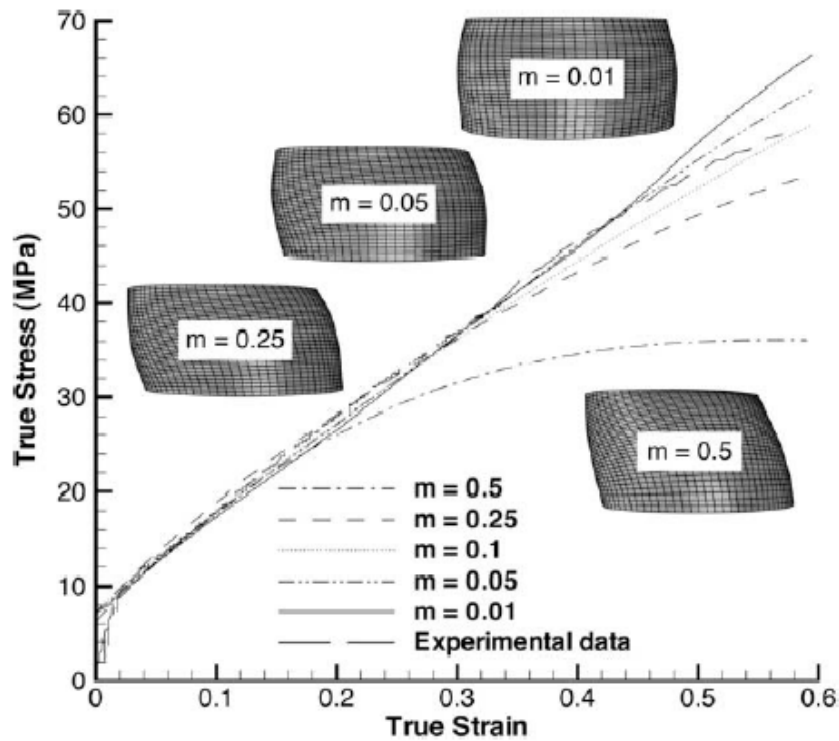
Cyberinfrastructure

IT technologies (hidden from the engineer) Conceptual design process (user-friendly interfaces) Engineering tools (CAD, CAE, etc.)

Click on image to enter

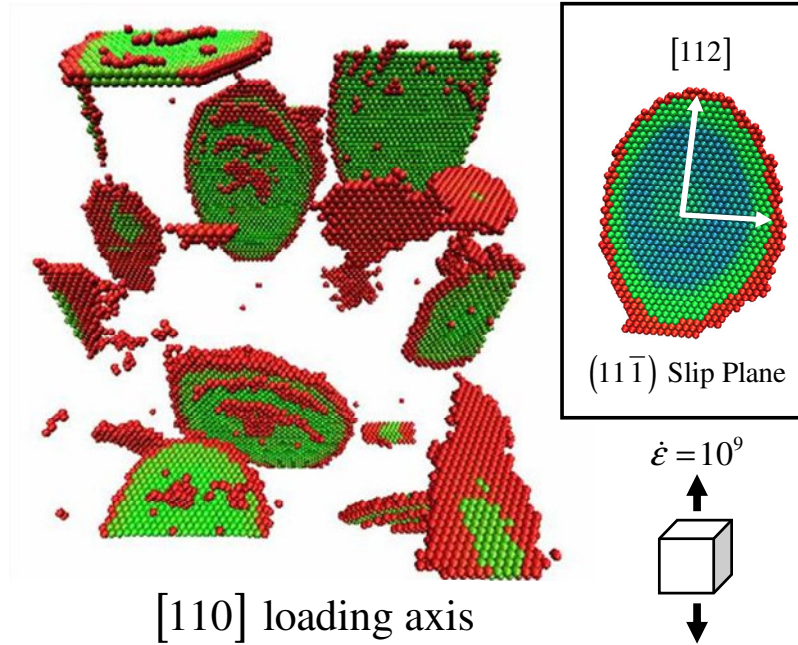
This page was last modified on 30 April 2010, at 14:54. This page has been accessed 799 times. [Privacy policy](#) [About EVOWiki](#)

Dislocation mobilities for Al multiscale models Groh, Marin, Horstemeyer, Zbib, IJP (2009)



Dislocation mobilities for AI multiscale models

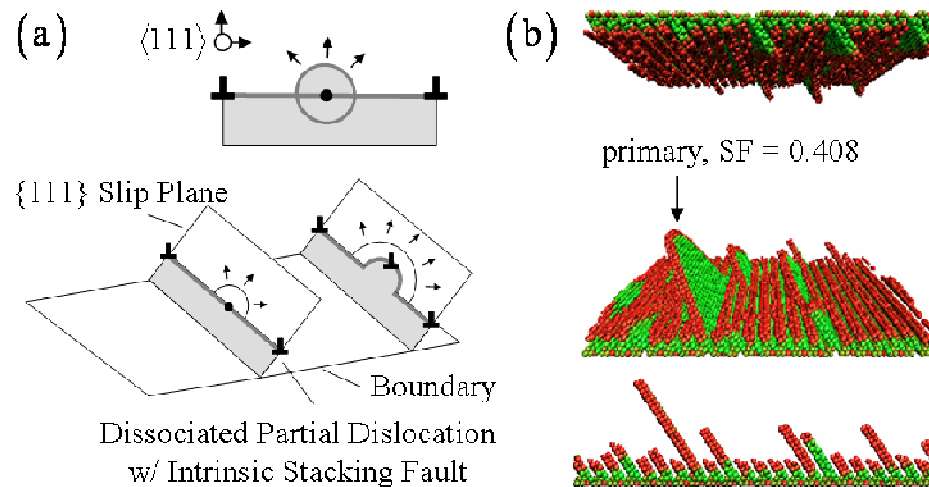
Single crystal dislocation nucleation Tschopp, McDowell, JMPS (2009)



Dislocation mobilities for AI multiscale models

Single crystal dislocation nucleation

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



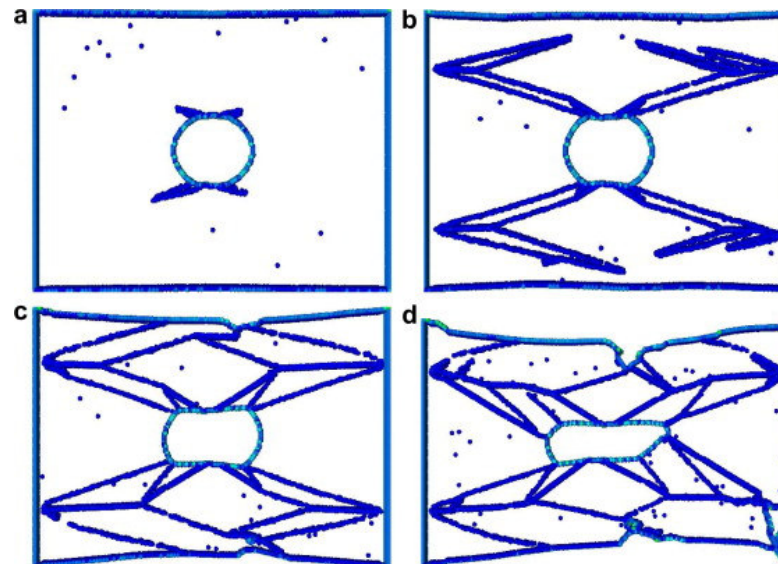
Dislocation mobilities for Al multiscale models

Single crystal dislocation nucleation

Grain boundary dislocation nucleation

Void growth and coalescence

Tang, Kim, Horstemeyer, *Acta Materialia* (2010)



Dislocation mobilities for Al multiscale models

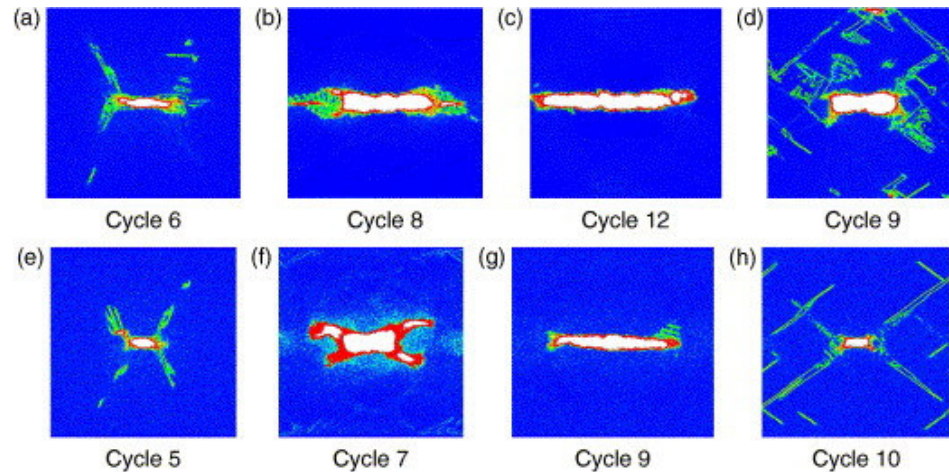
Single crystal dislocation nucleation

Grain boundary dislocation nucleation

Void growth and coalescence

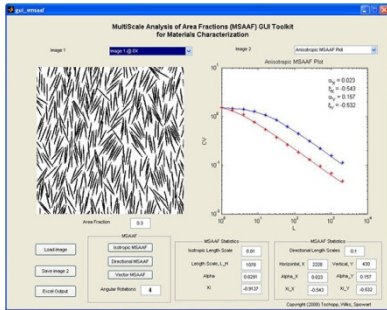
Fatigue and Damage

Potirniche, Horstemeyer, et al. IJF (2005)



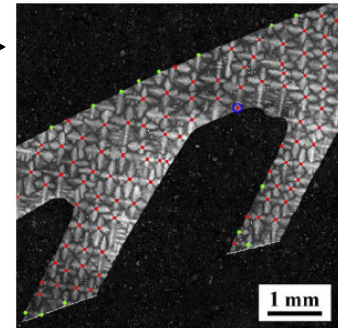
MATLAB Coupling w/ External Atomistic Codes

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

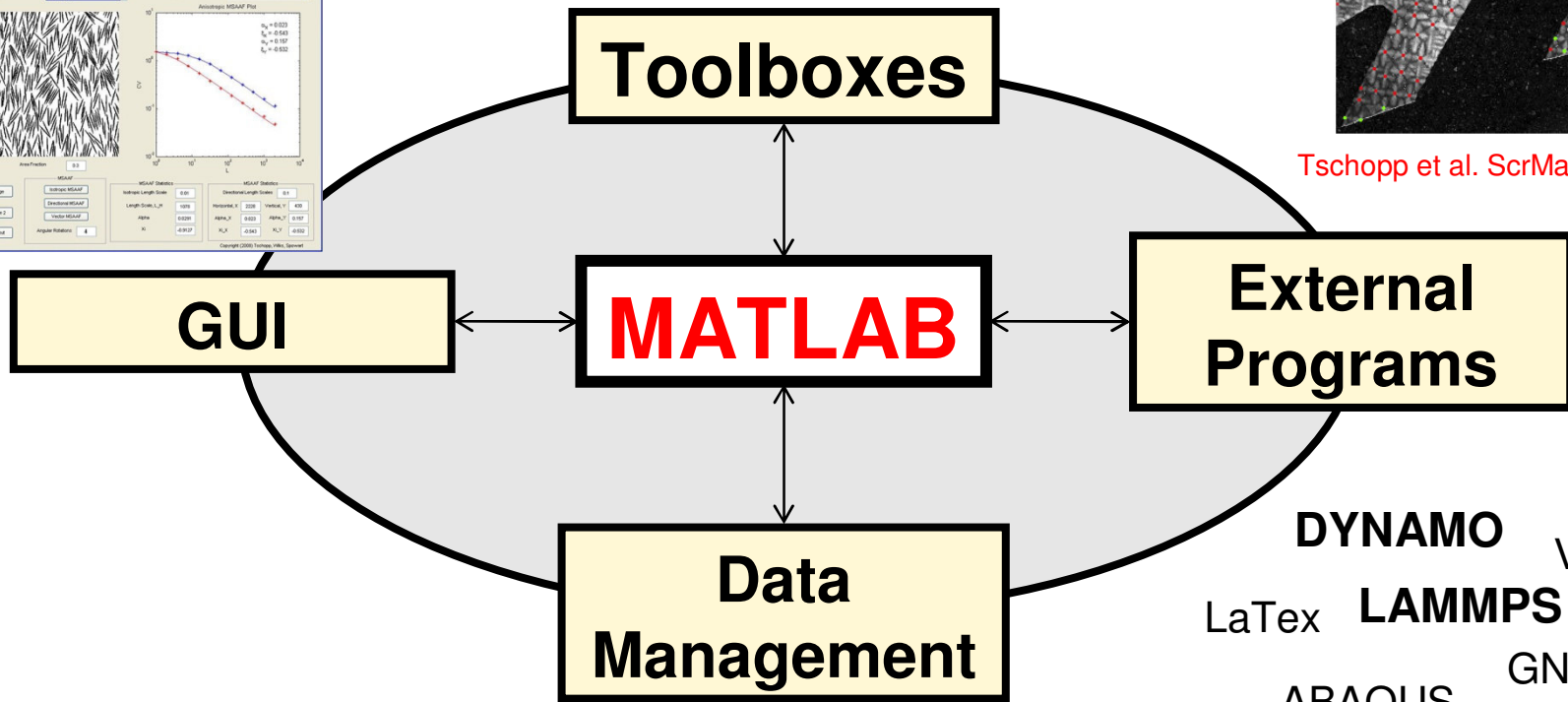


Spline Fitting Genetic Algorithm
Neural Network Image Processing →

Optimization Parallel Processing



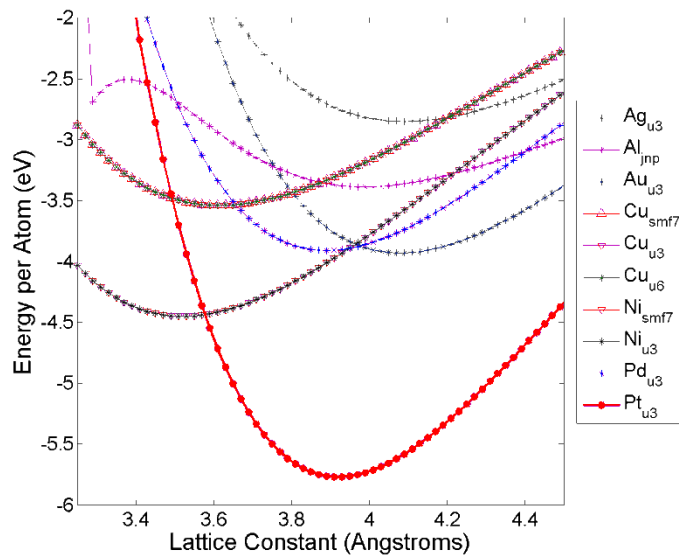
Tschopp et al. ScrMater (2010)



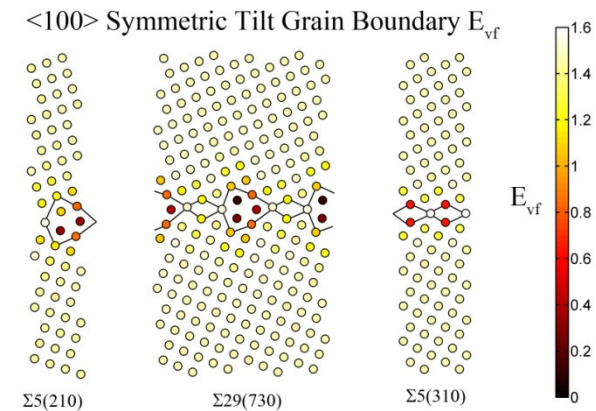
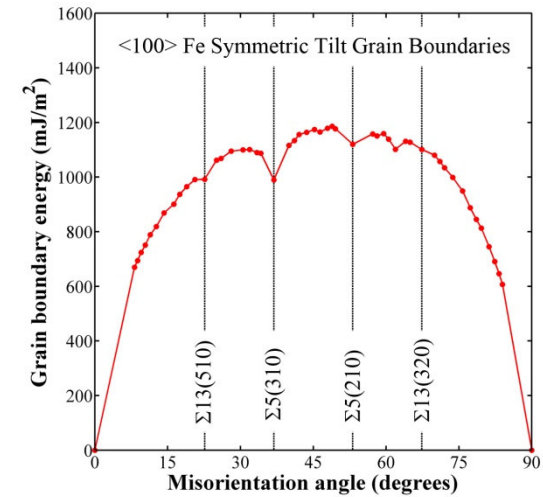
DYNAMO VASP
LaTex LAMMPS
ABAQUS GNUPLOT
VPSC

*.mat datafiles Write to Excel Output images
Generate LaTeX reports Write to *.ppt
*.fig graphs

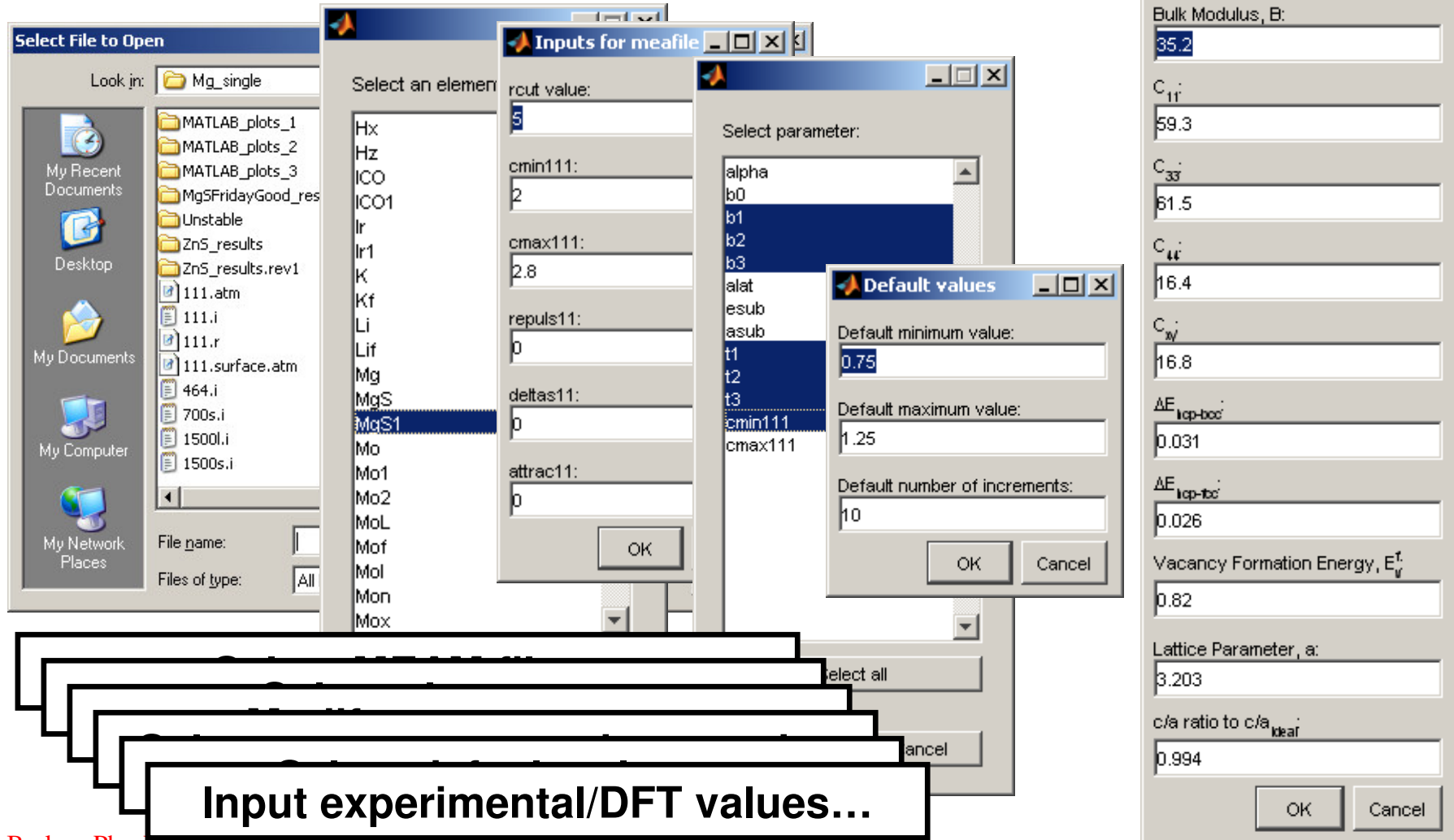
How do we generate the energy per atom for 10 different EAM potentials as a function of lattice constant? How do we do it quickly?



MATLAB coupled with
LAMMPS Windows
executable
(~70 sec for 250
simulations)



MEAM = Modified Embedded Atom Method^[1,2]

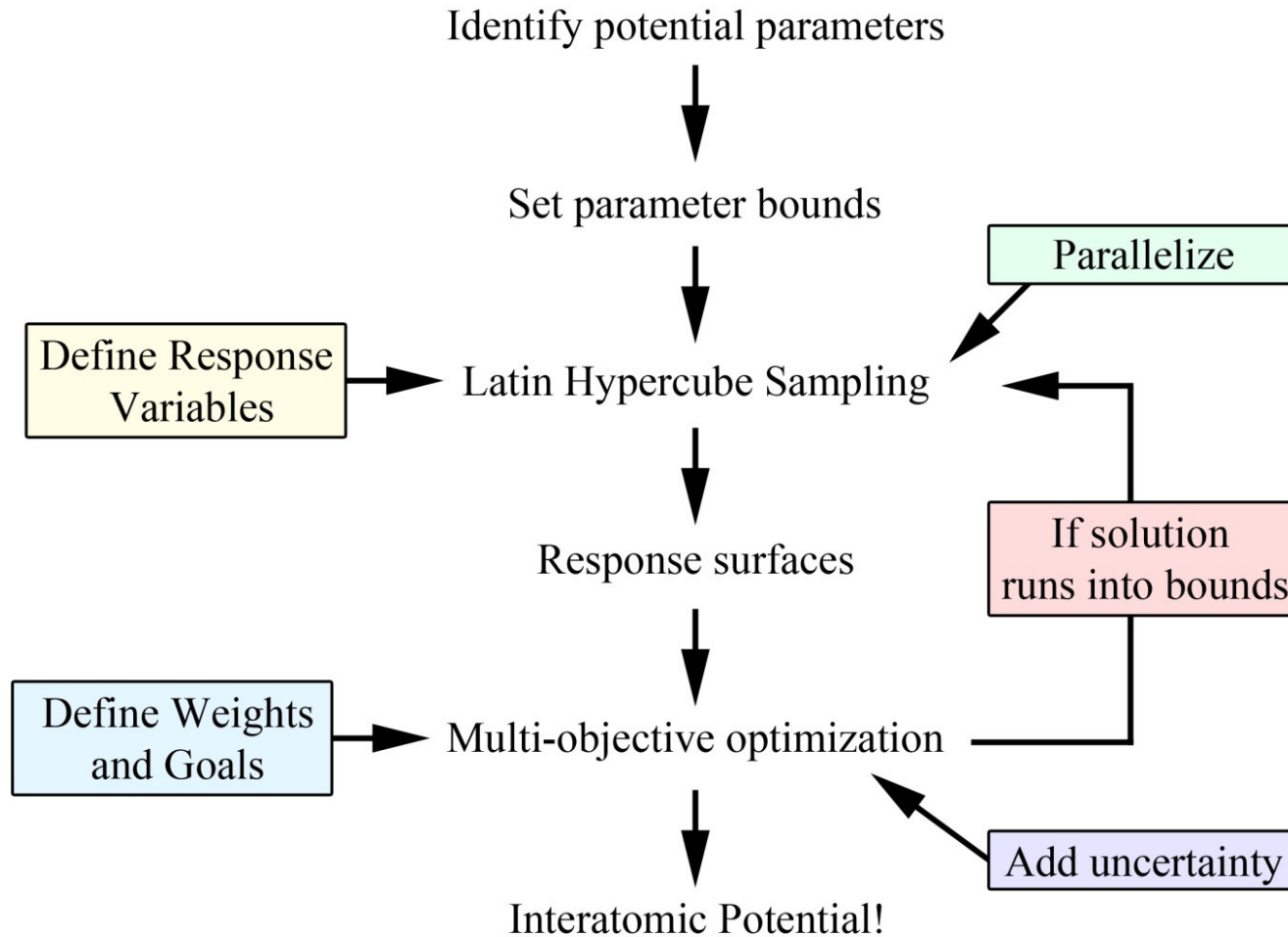


The image displays a series of overlapping software dialog boxes from the MEAM software. The primary dialog is 'Inputs for meamfile', which is used to define the input file for the MEAM potential. It includes fields for 'rcut value' (set to 5), 'cmin111' (2), 'cmax111' (2.8), 'repuls11' (0), 'deltas11' (0), and 'attrac11' (0). A 'Select parameter' list is visible, with 'cmin111' selected. A 'Default values' dialog box is also present, showing default values for 'Default minimum value' (0.75), 'Default maximum value' (1.25), and 'Default number of increments' (10). On the right, the 'Experimental/DF...' dialog box is shown, containing experimental values for Bulk Modulus (35.2), C₁₁ (59.3), C₃₃ (61.5), C₄₄ (16.4), C₁₂ (16.8), ΔE_{top-bcc} (0.031), ΔE_{top-fcc} (0.026), Vacancy Formation Energy, E_V^f (0.82), Lattice Parameter, a (3.203), and c/a ratio to c/a_{ideal} (0.994). A callout box at the bottom of the dialog boxes contains the text 'Input experimental/DFT values...'. The background shows a file explorer window with the 'Mg_single' directory selected, containing various files like '111.atm', '111.i', '111.r', '111.surface.atm', '464.i', '700s.i', '1500l.i', and '1500s.i'.

[1] Baskes, PhysRevB (1992)

[2] Baskes, Johnson, MSMSE (1994)

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



MEAM Interatomic Potential Development

Fe-He parameters

Single element MEAM parameters

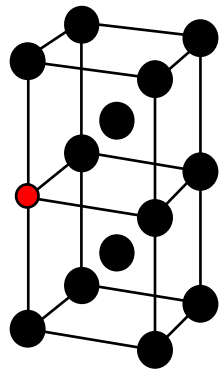
Parameter	Fe	He
alpha	5.027	8.350
alat	2.851	4.100
esub	4.280	0.032
asub	0.555	1
attrac/repuls11	0.150	0
rozero	1	0.450
Cmin111	0.8	2.0
Cmax111	1.9	2.8
b0	3.5	6.06
b1	2	6.06
b2	1	6.06
b3	1	6.06
t0	1	1
t1	-1.6	0
t2	12.5	0
t3	-1.4	0

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

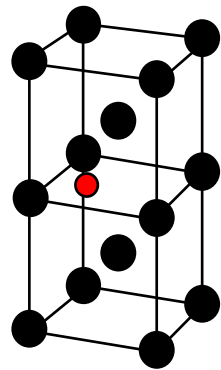
EAM

Fe-He response variables



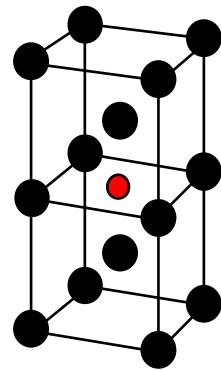
E_{sub}

4.00 eV



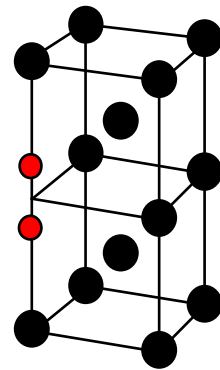
$E_{\text{tetrahedral}}$

4.37 eV



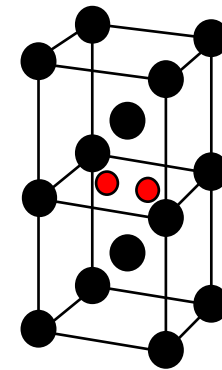
$E_{\text{octahedral}}$

4.60 eV



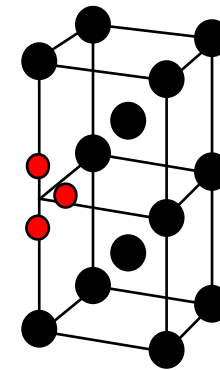
$E_{\text{He}_2\text{V}}$

6.61 eV



E_{He_2}

8.79 eV



$E_{\text{He}_3\text{V}}$

9.28 eV

Lowest energy in <100>

Didn't initially run...

INPUT

Single element
MEAM parameters

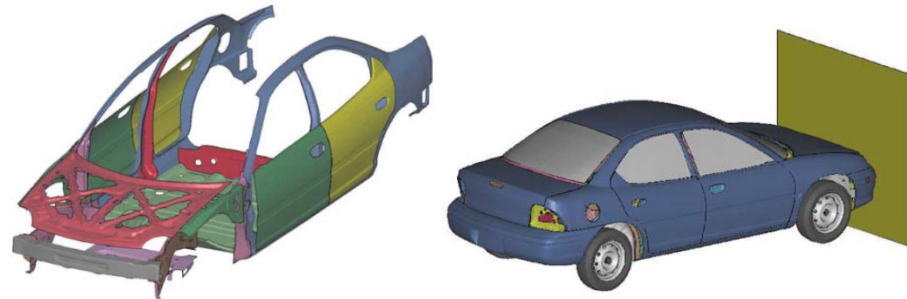
Parameter	Fe	He
alpha	5.027	8.350
alat	2.851	4.100
esub	4.280	0.032
asub	0.555	1
attrac/repuls11	0.150	0
rozero	1	0.450
Cmin111	0.8	2.0
Cmax111	1.9	2.8
b0	3.5	6.06
b1	2	6.06
b2	1	6.06
b3	1	6.06
t0	1	1
t1	-1.6	0
t2	12.5	0
t3	-1.4	0

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

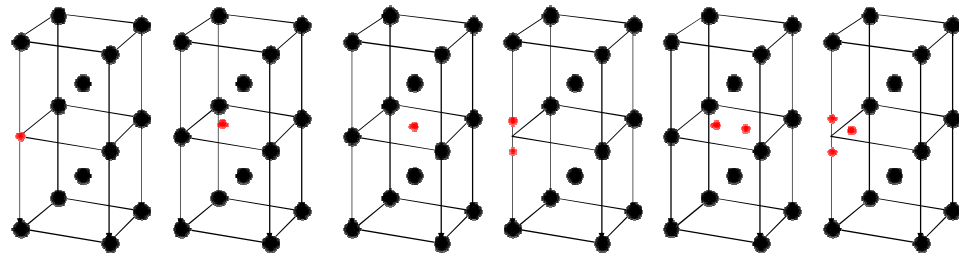
EAM

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



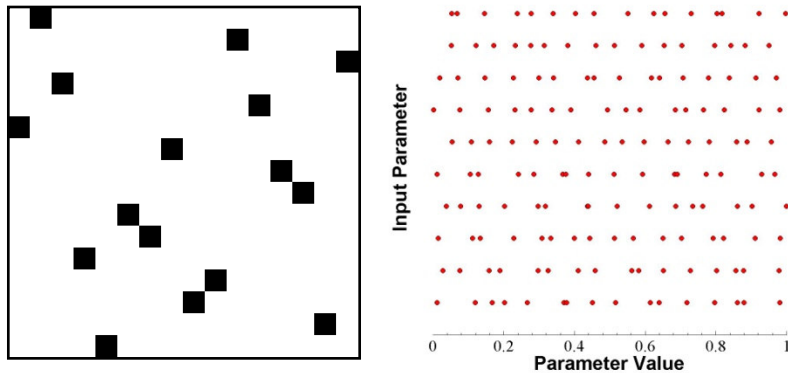
OUTPUT

Fe-He response variables



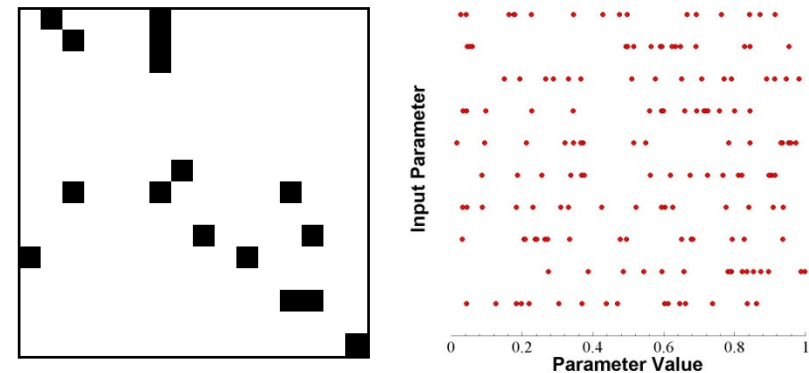
What is the most efficient way to sample n-dimensional parameter space?

LHS design



0 Parameter Space 1

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

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

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

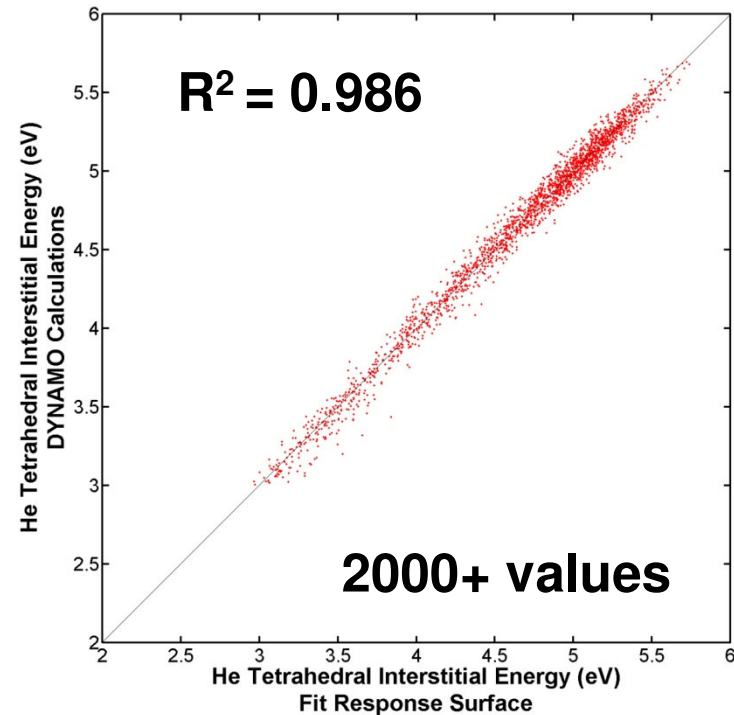
full quadratic

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

cubic

$$R^2 > 0.95$$

He Tetrahedral Interstitial Energy



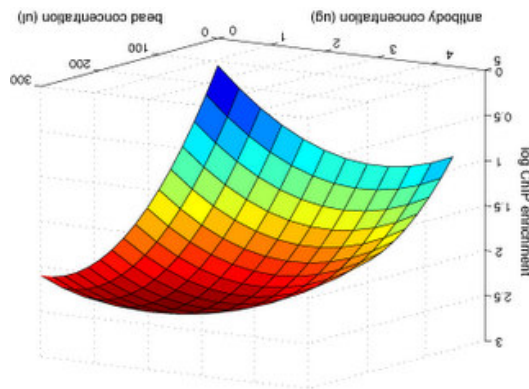
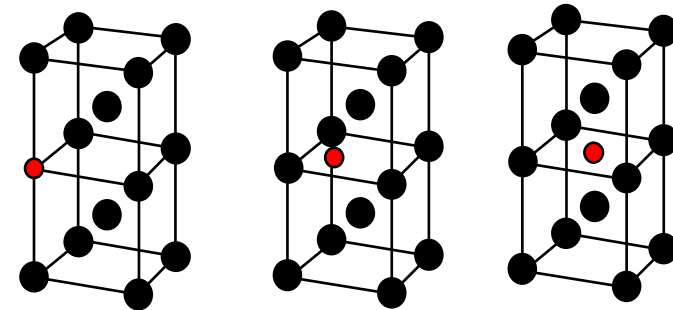
Response: 1 r2: 0.927, Response: 2 r2: 0.986
 Response: 3 r2: 0.997, Response: 4 r2: 0.995
 Response: 5 r2: 0.965, Response: 6 r2: 0.997

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

Min $F(x)$, such that

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

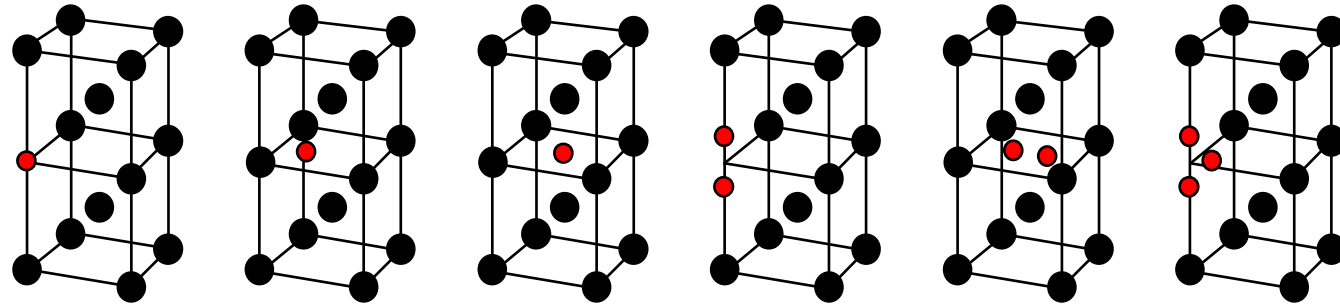
$$\sum_{i=1}^p W_i = 1, W_i > 0$$



	$E_{sub}(eV)$	$E_{tetra}(eV)$	$E_{octa}(eV)$
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



	$E_{\text{sub}}(\text{eV})$	$E_{\text{tetra}}(\text{eV})$	$E_{\text{octa}}(\text{eV})$	$E_{\text{He2V}}(\text{eV})$	$E_{\text{He2}}(\text{eV})$	$E_{\text{He3V}}(\text{eV})$
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

16,500 potentials sampled



$$E_{\text{He}_2\text{V},\langle 100 \rangle} < E_{\text{He}_2\text{V},\langle 110 \rangle}$$

$$E_{\text{He}_2\text{V},\langle 100 \rangle} < E_{\text{He}_2\text{V},\langle 111 \rangle}$$

$$E_{\text{He}_2} > 8 \text{ eV}$$

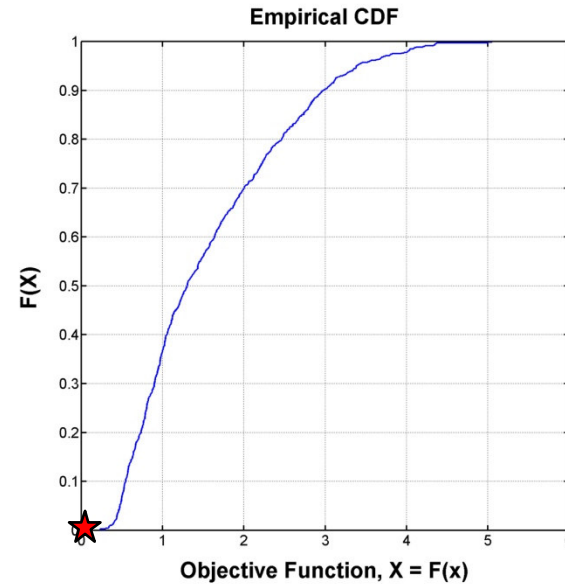
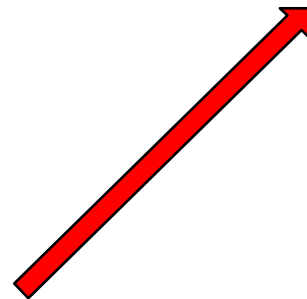
$$E_{\text{He}_3\text{V}} > 8 \text{ eV}$$



729 potentials

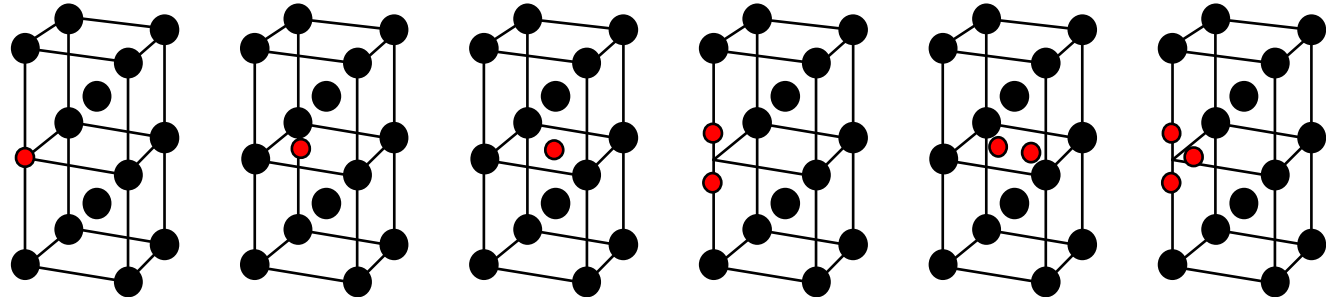


$$F(x) = \sum_{i=1}^p W_i (f_i(x) - g_i(x))^2$$



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

MEAM Interatomic Potential Development Fe-He parameters



	$E_{\text{sub}}(\text{eV})$	$E_{\text{tetra}}(\text{eV})$	$E_{\text{octa}}(\text{eV})$	$E_{\text{He2V}}(\text{eV})$	$E_{\text{He2}}(\text{eV})$	$E_{\text{He3V}}(\text{eV})$
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...?

- **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?