Intro

Metallic fuels

Gas swelling

Previous MD work on UZr

Previous work on metallic w/ Xe

What we will do

Computational Details

Potential background

DFT calculations

LAMMPS simulations

Results

Potential fitting

Matching DFT data

Xe int in bcc U vs T

Xe int in U-10Zr vs T

Xe-vac in bcc U vs T

Xe-vac in U-10Zr vs T

Xe bubble in U-10Zr: Same as the Xe in UMo/USi paper

Conclusion