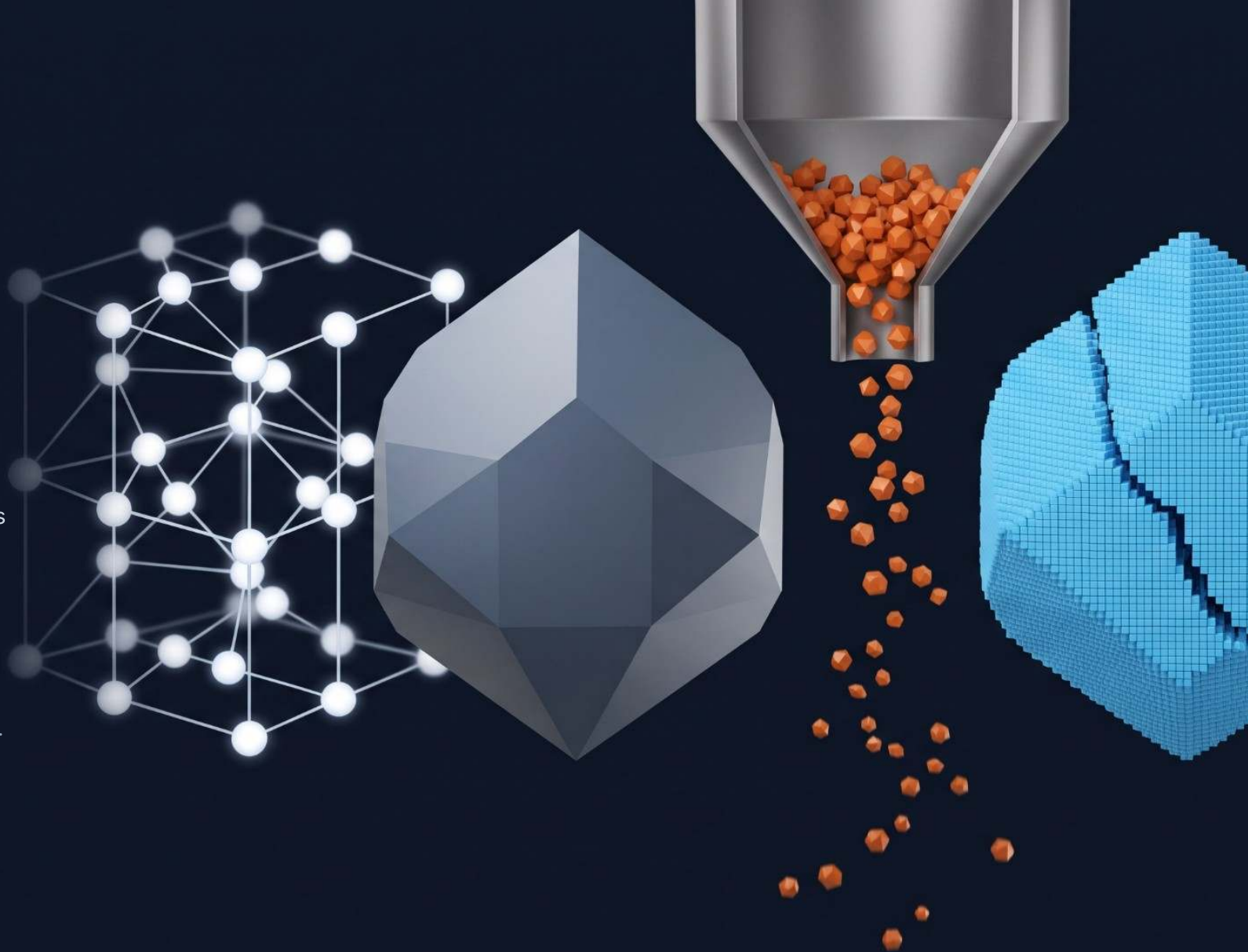


Atoms to Material

Simulation ready material properties from the crystal lattice, carried into GPU simulation of microstructures and process equipment.

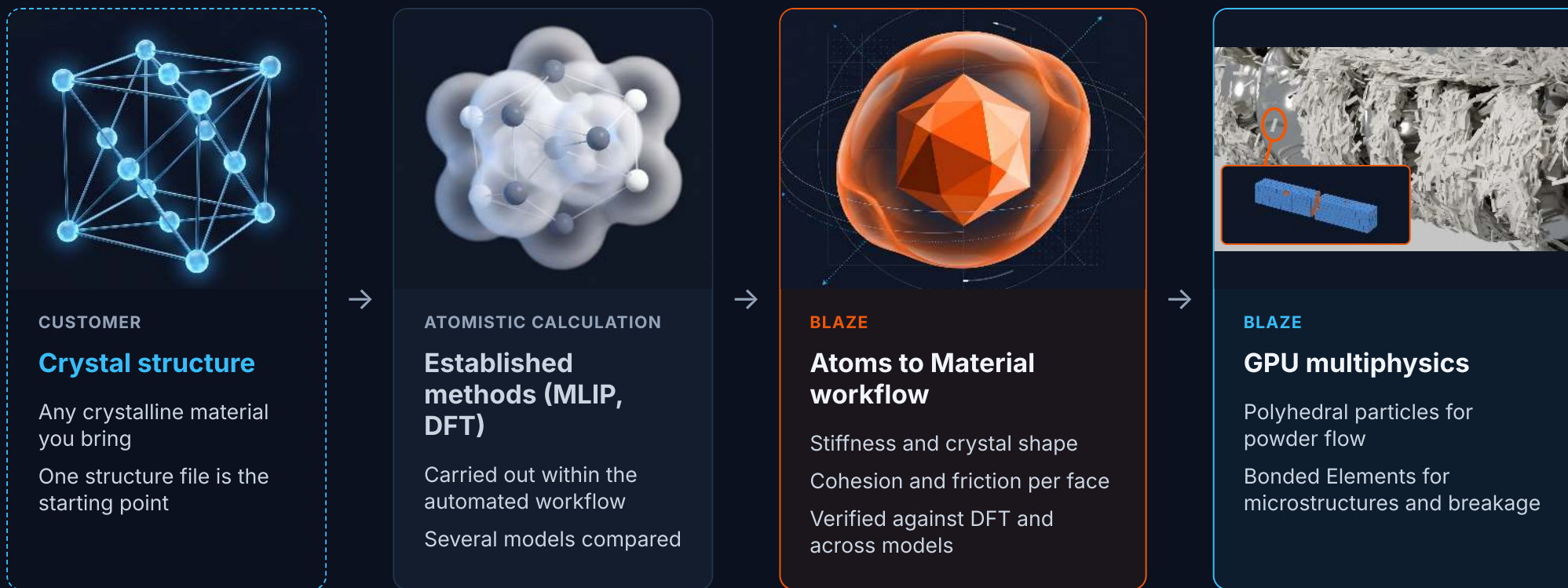
BYOL: Bring Your Own Lattice.

Blaze Computing · Ground truth for Physical AI.



From the lattice to the process

Process models are normally calibrated against bulk tests. Atoms to Material derives their inputs from the crystal structure.



Crystal form, particle shape and process settings **evaluated before manufacture.**

Value to development programmes



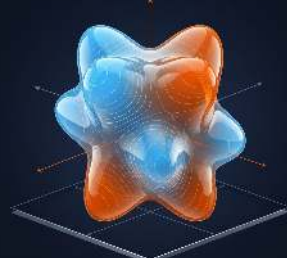
Early material data

Properties available at the lattice stage, before material exists in the quantities powder testing requires.



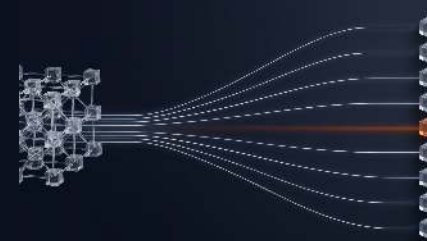
Simulation ready inputs

Elastic stiffness, crystal shape, and cohesion and friction per crystal face, delivered in solver format.



Full crystal anisotropy

All 21 elastic constants in every element, with cohesion and friction defined per particle face.



Traceable results

Verified against DFT, with the spread between models reported and every value labelled computed or calibrated.

One crystal, two routes

As a particle

Faceted particles with cohesion and friction per crystal face, for flow, feeding, hopper discharge and packing.



Equilibrium habit



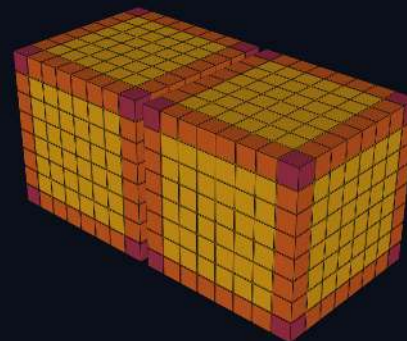
Needle



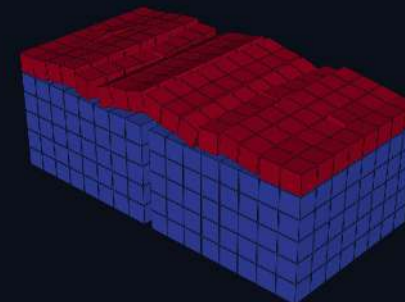
Lath

As a bonded body

Each element carries the full crystal stiffness. Cracks initiate at internal defects, and a brittle coating fails before the underlying alloy. Fragments separate and interact in the same solver.



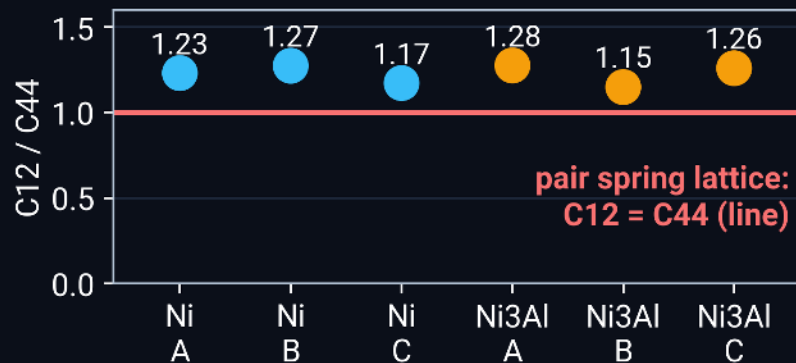
Central void



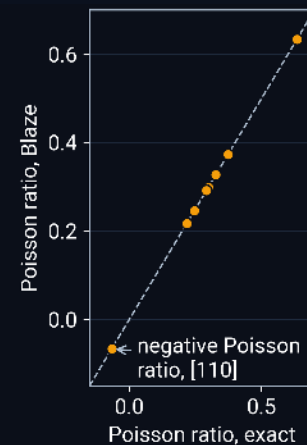
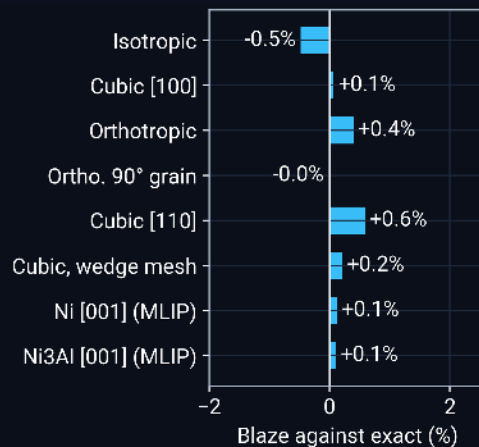
Brittle coating on an alloy

A stress law, not springs

Each bonded Element carries the full crystal stiffness and orientation, verified against exact anisotropic elasticity in the regression suite.



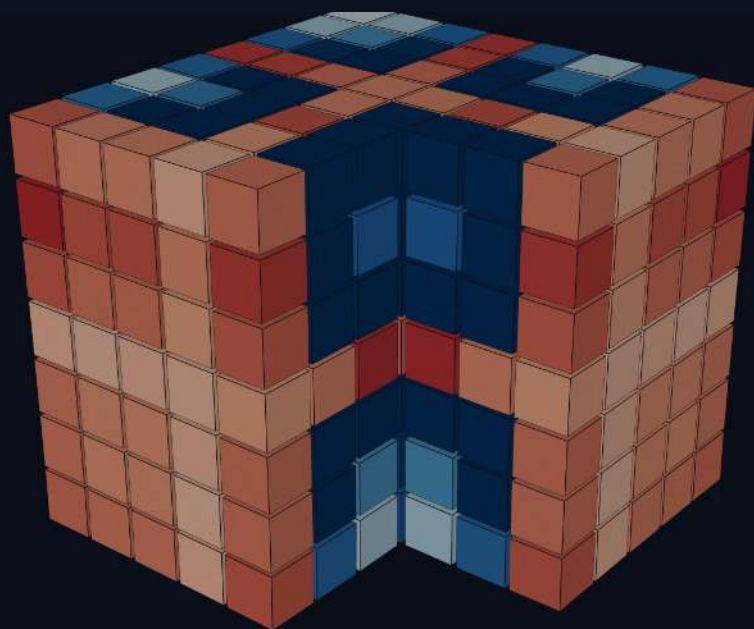
Central pair spring lattices are limited to $C_{12} = C_{44}$; the computed alloy crystals have C_{12} / C_{44} of 1.15 to 1.28.



Modulus within 1 % and Poisson ratio within 0.005 of exact anisotropic elasticity, including the negative Poisson ratio of a cubic crystal along [110].

Worked example: alloy microstructure

Ni / Ni₃Al: 42 % γ' cubes in γ channels, 512 bonded hex elements, the stiffness of each phase computed from its lattice.



138.7 GPa

[001] modulus, within the Reuss and Voigt bounds of the phases (136.7 to 140.2 GPa).

0.35 %

Deviation from a continuum (FE) reference of the same body.

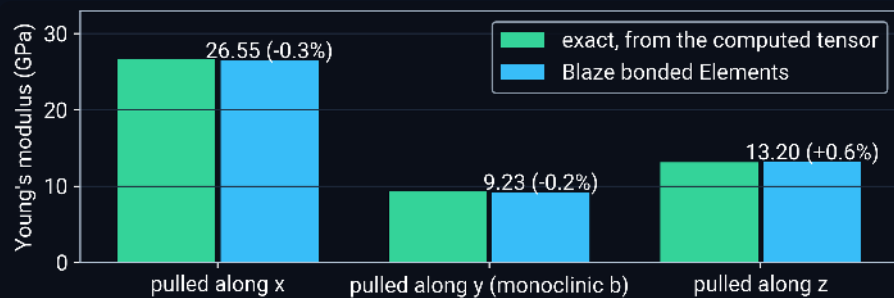
Misfit as eigenstrain

γ' held in compression (blue), γ channels in tension (red).

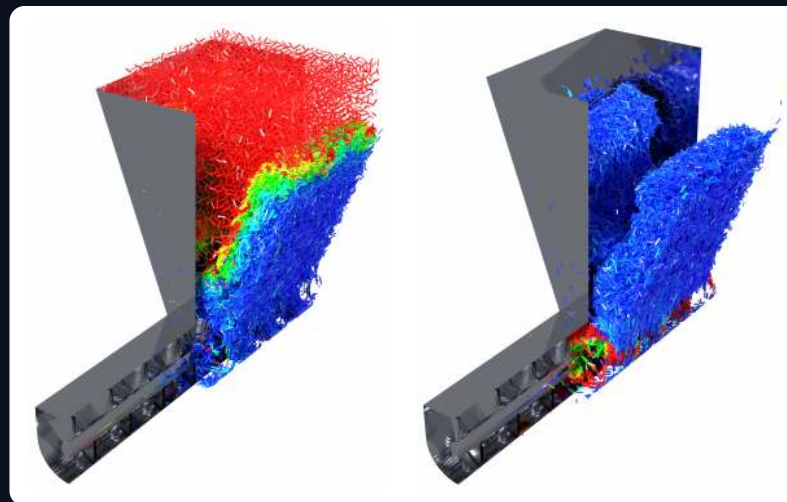
Misfit of the 0 K binary phases, used as a demonstration input.

Worked example: API crystal to process equipment

Paracetamol form I. Density, stiffness, crystal shape and per face cohesion are derived from the crystal rather than fitted to angle of repose tests.



A bonded Element crystal reproduces the monoclinic stiffness on all three axes within 0.6 %. Bulk and shear moduli are within 2 % of dispersion corrected DFT.



Screw feeder model with crystal derived particles: hopper filling (left) and cohesive powder retained on the hopper walls (right).

Computed from the lattice, calibrated once per material class

Computed from the lattice

Density	Crystal shape
Stiffness tensor, 21 constants	Particle cohesion
Surface energy of each crystal face	Lattice misfit

Calibrated once per material class

Fracture strength of bonded Elements	Fracture energy of bonded Elements
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Polyhedral contact

Volume based contact for faceted crystals and fragments.

One GPU solver

Bonded Elements fracture into particles alongside SPH fluids and CFD.

Open to learned models

Element stress and strain in GPU memory, accessible from Python.

BYOL: Bring Your Own Lattice.

Start from the crystal structure of your material.

director@blazecomputing.co.uk

www.blazecomputing.co.uk

Ground truth for Physical AI.



NVIDIA CUDA Research Center since 2013 (Blaze-DEM, University of Johannesburg); NVIDIA Applied Research Accelerator Program; NVIDIA Inception Program member.