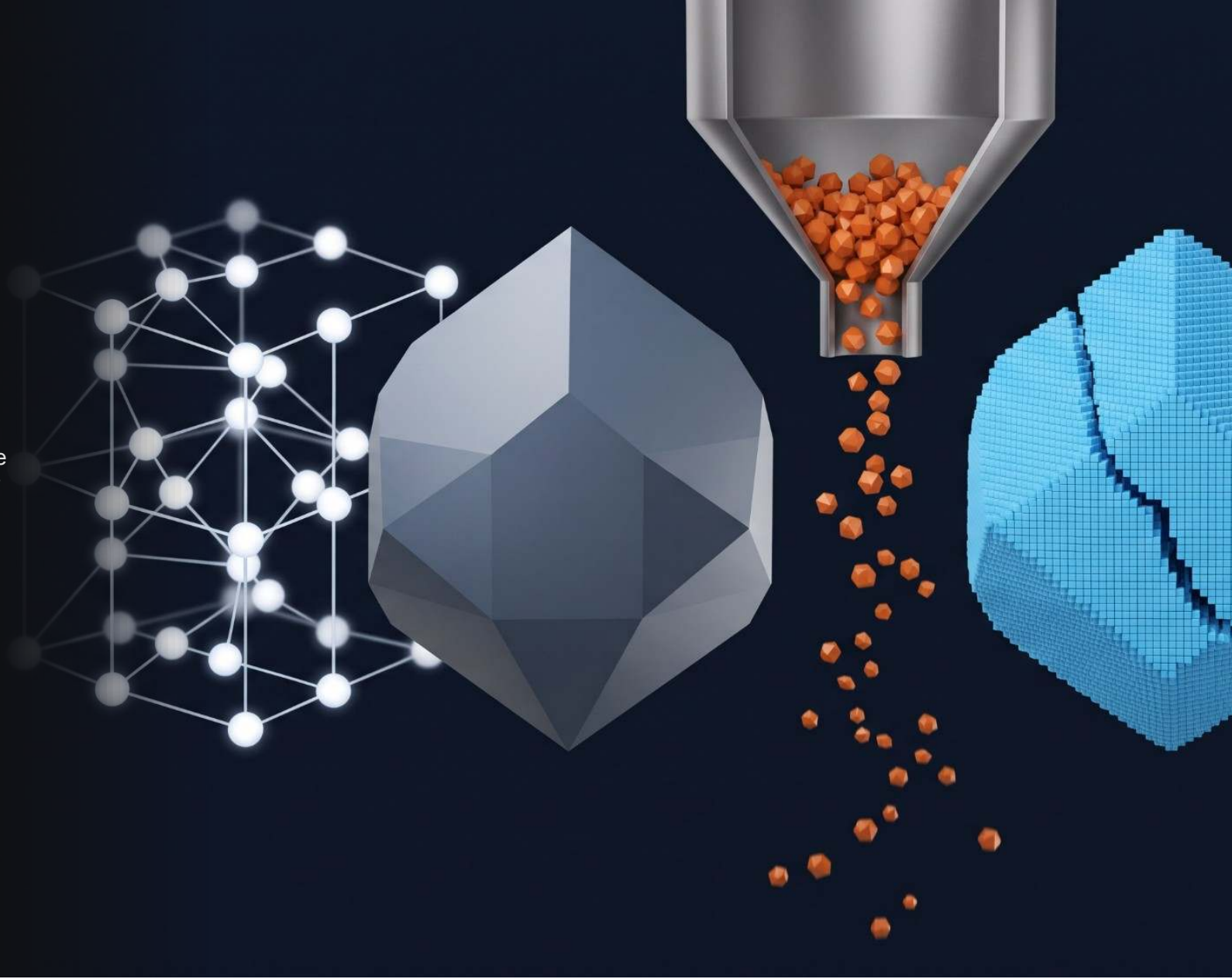
Atoms to Material

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

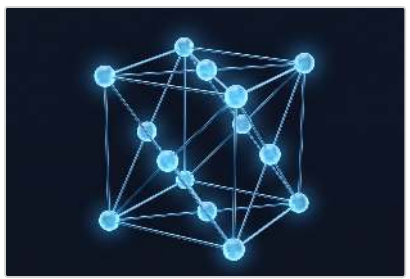
BYOL: Bring Your Own Lattice.

Blaze Computing · Ground truth for Physical AI.

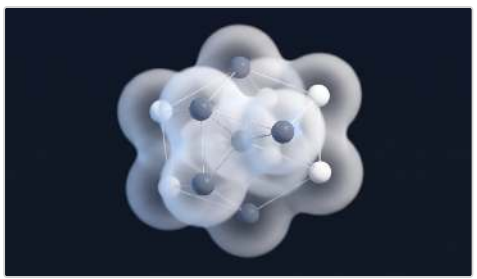


From the lattice to the process

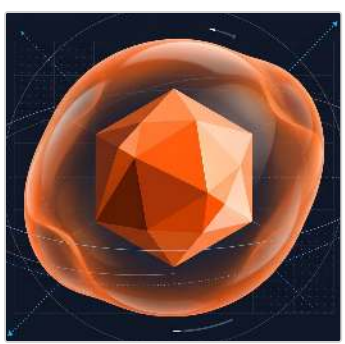
Process models are normally calibrated against bulk tests. Atoms to Material derives their inputs from the crystal structure.



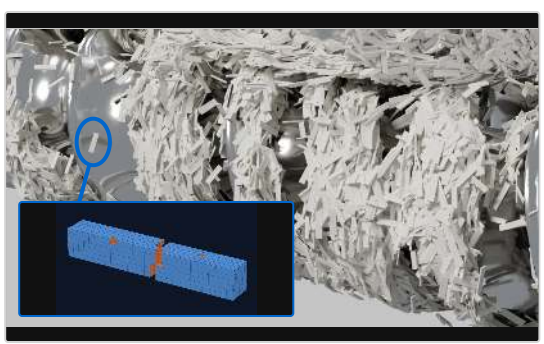
1. Crystal structure



2. Established methods (MLIP, DFT)



3. Atoms to Material workflow



4. GPU multiphysics

Stage	What happens
1. Crystal structure Customer	Any crystalline material you bring One structure file is the starting point
2. Established methods (MLIP, DFT) Atomistic calculation	Carried out within the automated workflow Several models compared
3. Atoms to Material workflow Blaze	Stiffness and crystal shape Cohesion and friction per face Verified against DFT and across models
4. GPU multiphysics Blaze	Polyhedral particles for powder flow Bonded Elements for microstructures and breakage

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

Value to development programmes



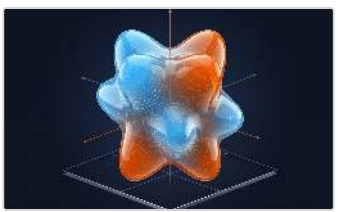
Early material data

Material properties at the lattice stage, before bulk powder tests.



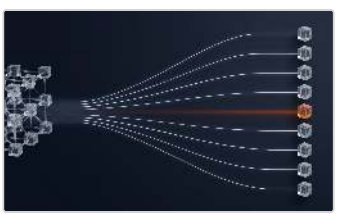
Simulation ready inputs

Stiffness, crystal shape, cohesion and friction in solver format.



Full crystal anisotropy

All 21 elastic constants per element, cohesion and friction per face.



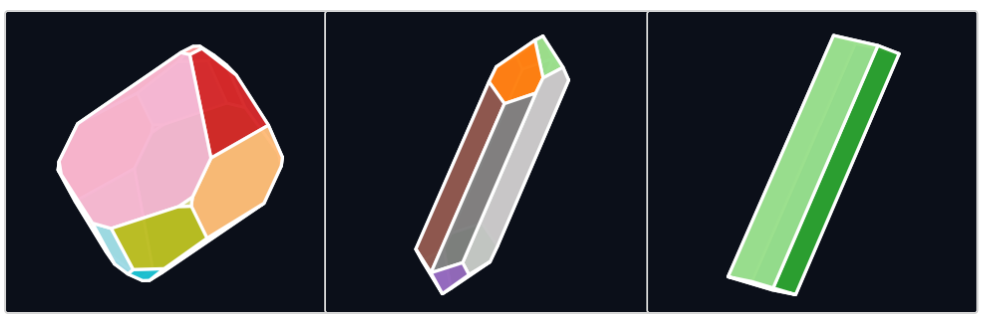
Traceable results

Checked against DFT, model spread reported, every value labelled.

One crystal, two routes

As a particle

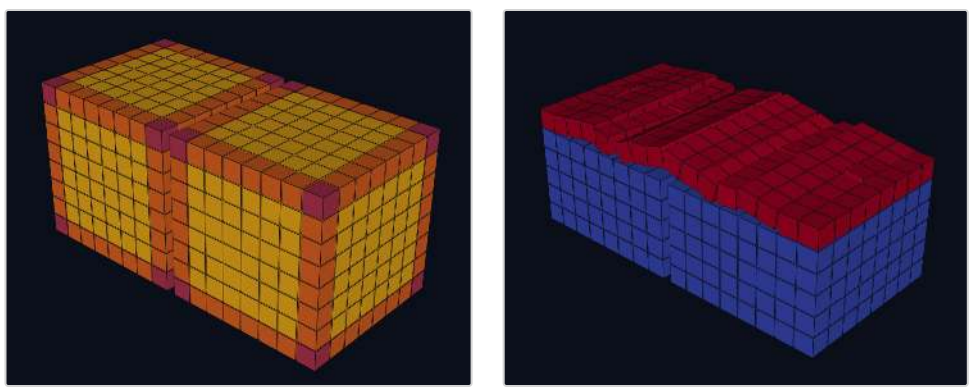
Faceted particles with cohesion and friction per crystal face, for flow, feeding, hopper discharge and packing.



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.



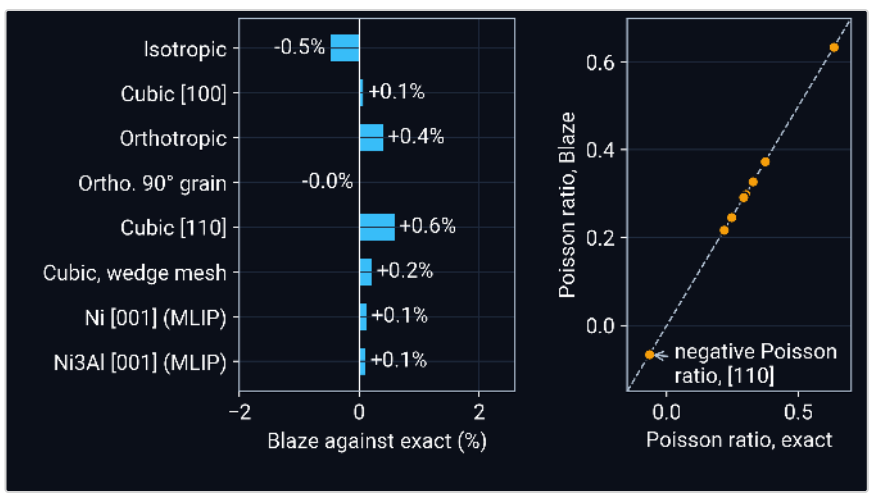
Central void | Brittle coating on an alloy

A stress law, not springs

Each bonded Element carries the full crystal stiffness and orientation, verified within 1 % in modulus and 0.005 in Poisson ratio against exact anisotropic elasticity.



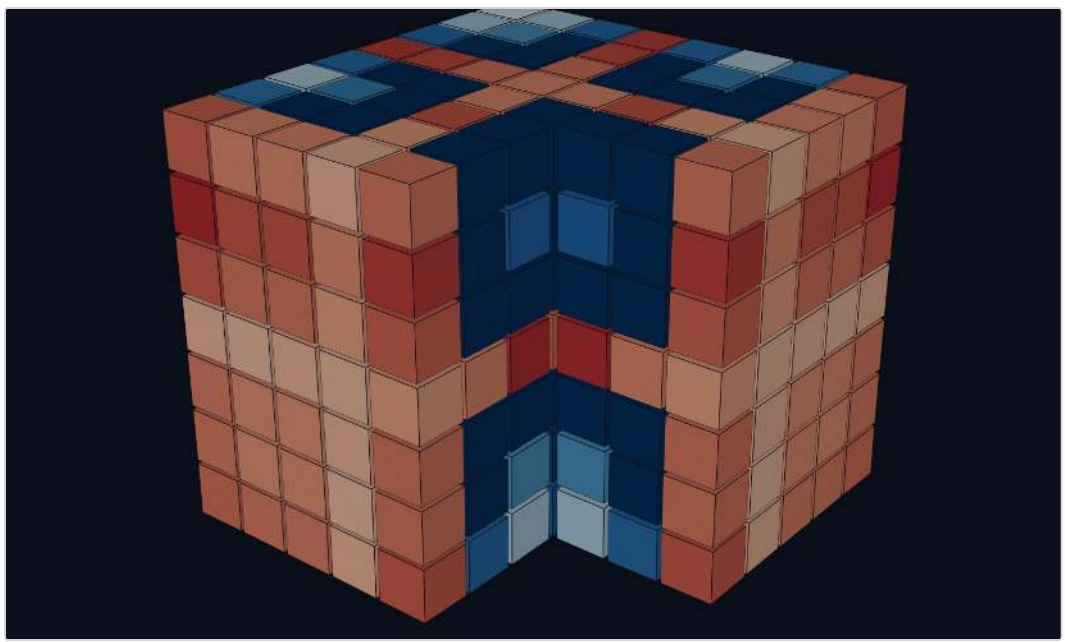
Alloy elastic ratio against the pair spring limit.



Bonded Elements checked against exact anisotropic elasticity.

Worked example: alloy microstructure

Ni / Ni_3Al: 42 % γ′ cubes in γ channels, 512 bonded hex elements, the stiffness of each phase computed from its lattice.



Check	Result
[001] modulus	**138.7 GPa**, within the Reuss and Voigt bounds of the phases (136.7 to 140.2 GPa).
Continuum (FE) check	**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).

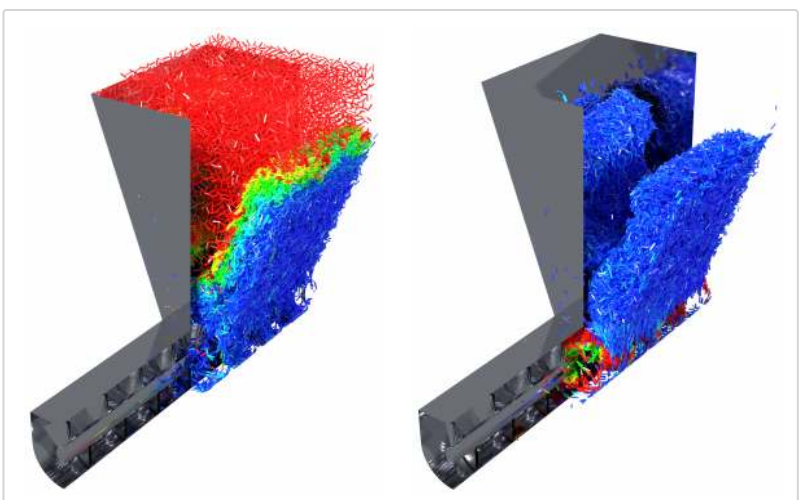
Misfit of the 0 K binary phases, used as an example input.

Worked example: API crystal to process equipment

Paracetamol form I: properties derived from the crystal rather than angle of repose fitting (stiffness within 0.6 % on three axes, DFT moduli within 2 %).



Monoclinic stiffness of a paracetamol crystal in Blaze.



Needle paracetamol crystals in a screw feeder.

Computed from the lattice, calibrated once per material class

Source	Properties	
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

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.