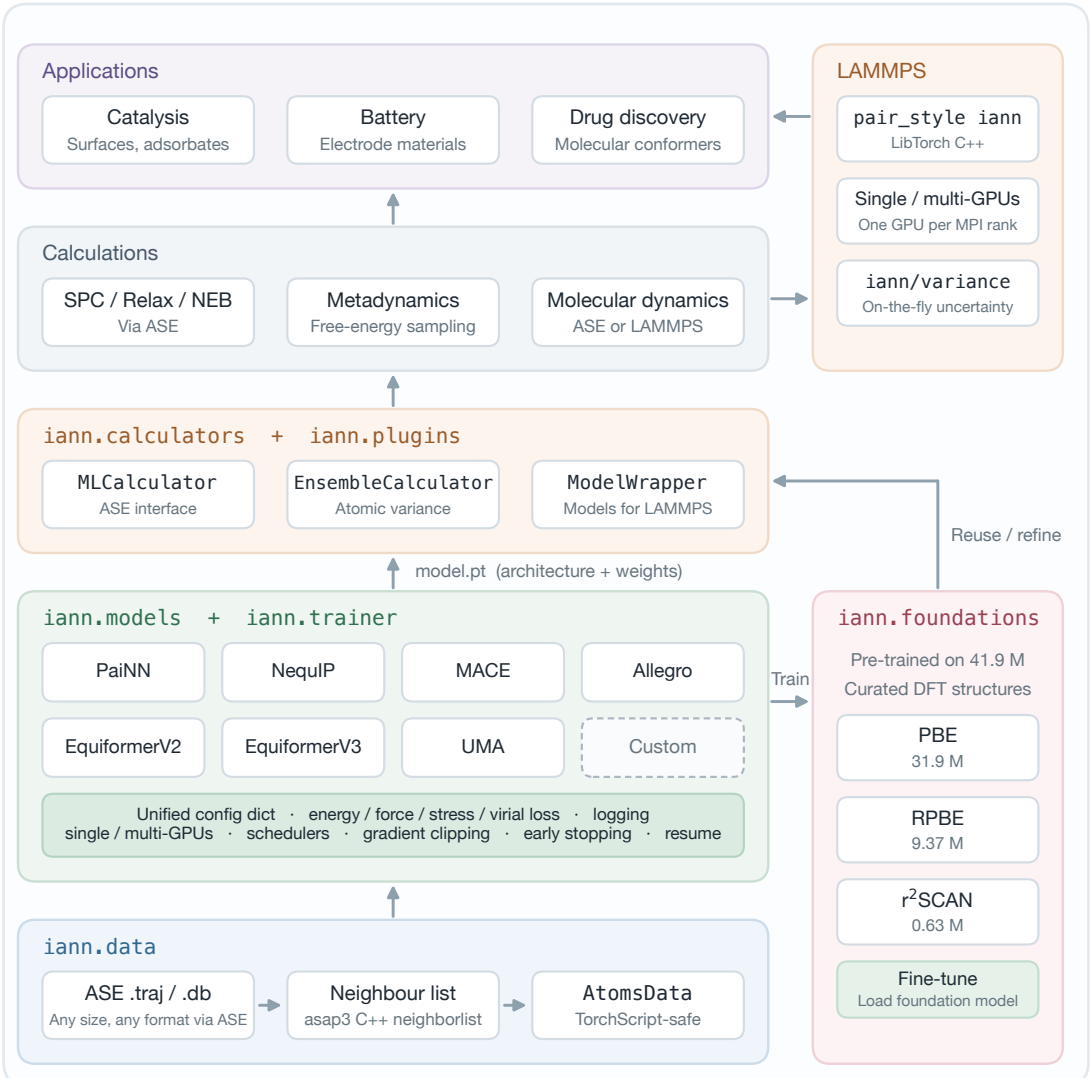

Applications
Catalysis
Surfaces, adsorbates
Battery
Electrode materials
Drug discovery
Molecular conformers
LAMMPS
pair_style iann
LibTorch C++
Single / multi-GPUs
One GPU per MPI rank
iann/variance
On-the-fly uncertainty
Calculations
SPC / Relax / NEB
Via ASE
Metadynamics
Free-energy sampling
Molecular dynamics
ASE or LAMMPS
iann.calculators + iann.plugins
MLCalculator
ASE interface
EnsembleCalculator
Atomic variance
ModelWrapper
Models for LAMMPS
Reuse / refine
model.pt (architecture + weights)
iann.models + iann.trainer
PaiNN
NequIP
MACE
Allegro
EquiformerV2
EquiformerV3
UMA
Custom
Unified config dict · energy / force / stress / virial loss · logging
single / multi-GPUs · schedulers · gradient clipping · early stopping · resume
Train
iann.foundations
Pre-trained on 41.9 M
Curated DFT structures
PBE
31.9 M
RPBE
9.37 M
r2SCAN
0.63 M
Fine-tune
Load foundation model
iann.data
ASE .traj / .db
Any size, any format via ASE
Neighbour list
asap3 C++ neighborlist
AtomsData
TorchScript-safe