CompuTherm, LLC
8401 Greenway Blvd
Suite 248
Middleton, WI 53562
USA

Phone +1 (608) 203-8843
Fax +1 (608) 203-8045
Email info@computherm.com
Web www.computherm.com

CompuTherm Newsletter

September, 2026

Introducing PandatAi and Pandat™ 2026A

Bringing CALPHAD, ICME, and AI together for smarter materials design

CompuTherm is pleased to introduce PandatAi, a new AI-powered materials design platform, and to announce the release of Pandat 2026A.

- **PandatAi** provides an intelligent platform for AI-assisted materials design and CALPHAD/ICME workflow automation.
- **Pandat 2026A** expands Pandat's solidification and microstructure simulation capabilities with two new PanPhaseField plugins.

This newsletter highlights both developments and shows how they extend CompuTherm's capabilities in materials design, process simulation, and ICME.

PandatAi: AI-Powered Materials Design Platform

PandatAi is designed to help users move from materials questions to CALPHAD/ICME-based computational workflows. Instead of manually setting up every calculation, users can describe what they want in plain language. PandatAi can help design the calculation, select appropriate settings, run the task through PandatX, generate plots, interpret results, and organize the study into a technical report.

PandatAi can support a wide range of materials design workflows, including phase diagram calculations, solidification simulations, precipitation and microstructure evolution, diffusion, high-throughput screening, and broader ICME applications. Users can also create and add custom workflows into PandatAi to accelerate materials design.

For new users, PandatAi lowers the learning barrier. For experienced users, it improves productivity by making multi-step studies faster and easier to organize.

An introductory video is available on YouTube: PandatAi: AI-Powered Materials Design Platform

CompuTherm, LLC
8401 Greenway Blvd
Suite 248
Middleton, WI 53562
USA
Phone +1 (608) 203-8843
Fax +1 (608) 203-8045
Email info@computherm.com
Web www.computherm.com

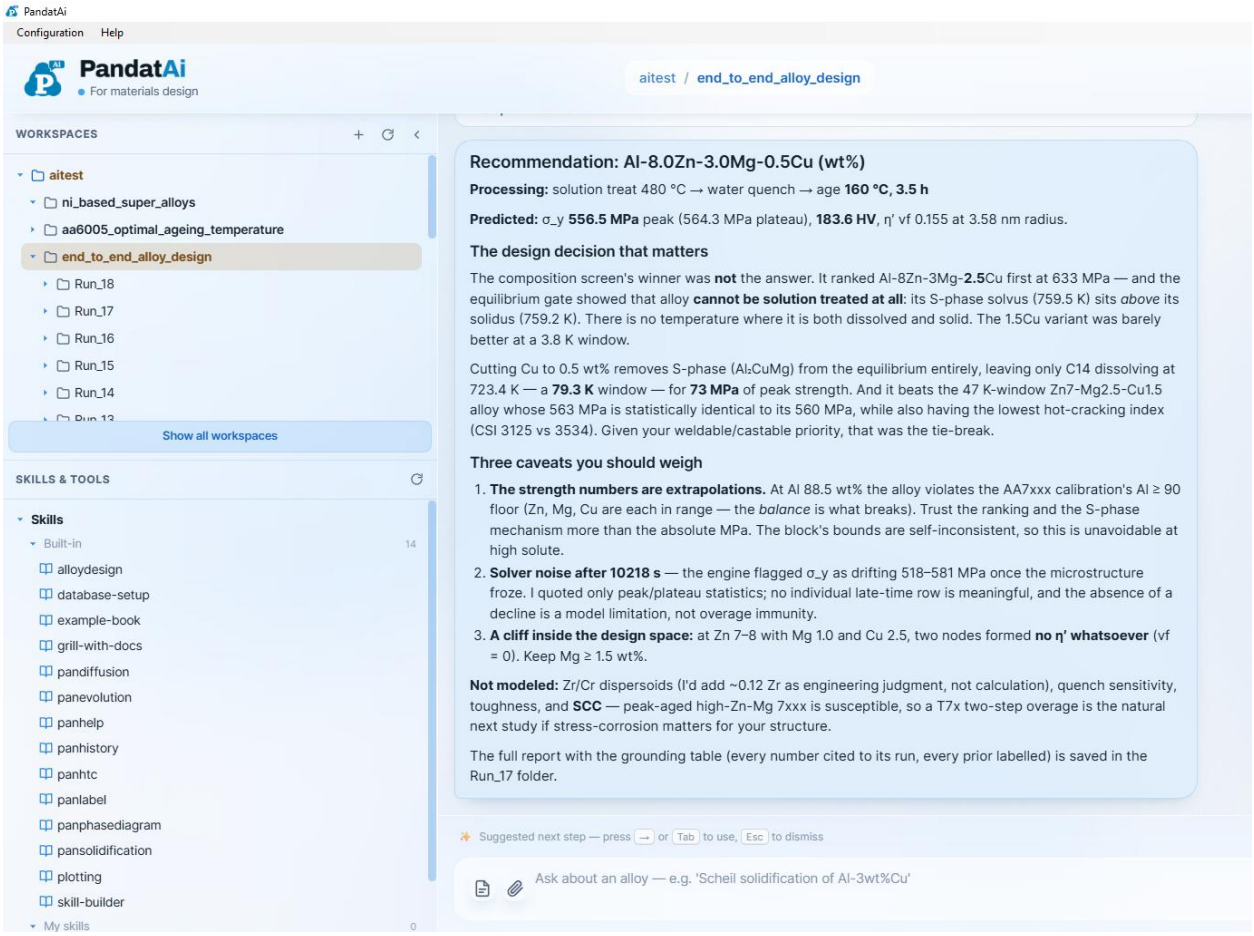

Fig. 1: PandatAi in an end-to-end alloy design study.

Figure 1 illustrates an example in which, starting from a user's plain-language request, PandatAi automatically performs equilibrium calculations and precipitation simulations to identify a recommended alloy composition and appropriate solution-treatment and aging schedule for achieving optimal strength and hardness in an aluminum alloy. A comprehensive report containing all simulation results and procedures is recorded in the PandatAi workspace, allowing users to trace the details of the analysis and understand the rationale behind the final recommendations.

CA Solidification Plugin: Grain Structure Prediction Inside Pandat

Pandat 2026A introduces a CA Solidification Plugin in PanPhaseField module. This plugin significantly enhances the capability of Pandat for solidification simulation. This plugin enables the simulation of grain nucleation, growth, impingement, grain size, grain shape, crystal orientation, and columnar-to-equiaxed transition during casting, welding, and additive manufacturing processes.

The CA model is coupled with Pandat's CALPHAD engine, so microstructure evolution is driven by alloy-specific thermodynamic and solidification behavior.

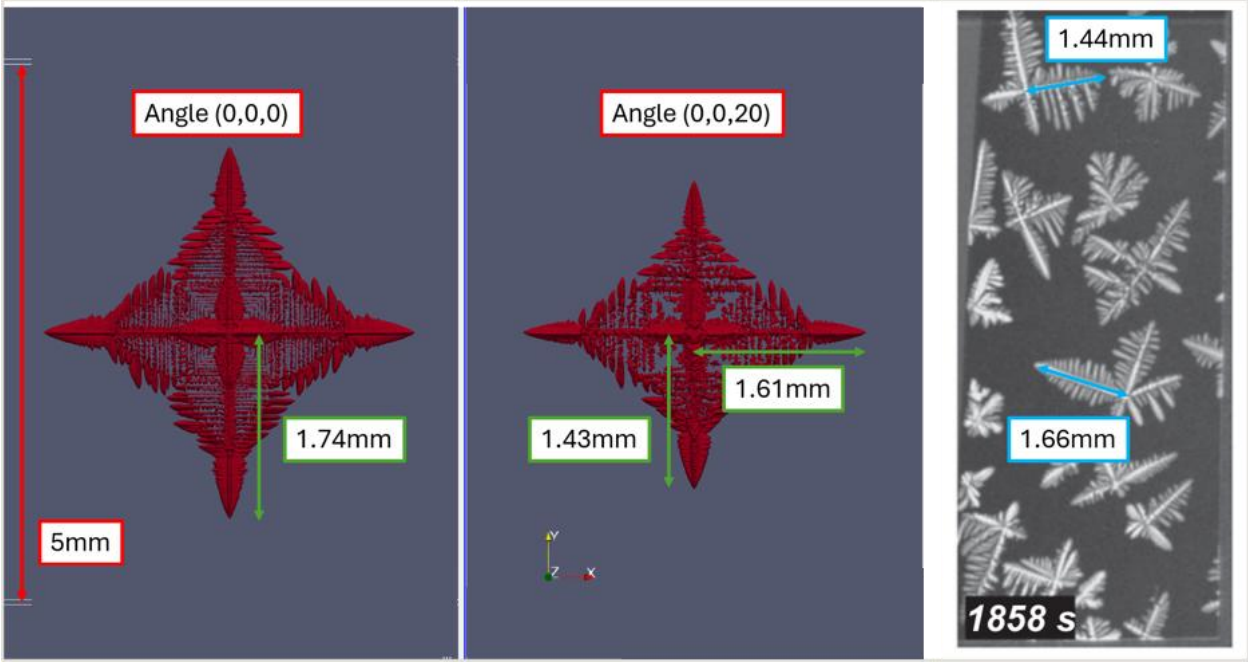

Fig. 2: Simulated dendrite in Al-10Cu (wt%) for a 0.5 K/min cooling rate using the CA Solidification Plugin. The last micrograph is a comparison with the experiment [2009Bogno].

OP Solidification Plugin: Multicomponent Phase-Field Solidification

Pandat 2026A also includes the OP Solidification Plugin, built on the OpenPhase framework [2017Tegeler] and integrated with Pandat's CALPHAD engine. This plugin supports multicomponent, multiphase solidification simulations with live thermodynamic coupling. Key quantities such as tie lines, partition coefficients, chemical driving forces, and multicomponent diffusivities can be queried from Pandat during the simulation rather than relying on pre-tabulated approximations.

Beyond this live thermodynamic coupling, the plugin models anisotropic interface energy and mobility with stochastic nucleation, going beyond binary or ternary approximations, and captures multicomponent diffusional interactions through a full diffusivity matrix (cross diffusion) for realistic microsegregation. In addition, the plugin can also simulate directional solidification under a given cooling rate and thermal gradient as shown in Figure 3. By adopting a multi-phase field model, the plugin supports multi-phase simulations of both eutectic and peritectic solidification.

This provides a powerful new approach for studying realistic solidification and microsegregation behavior in complex alloys.

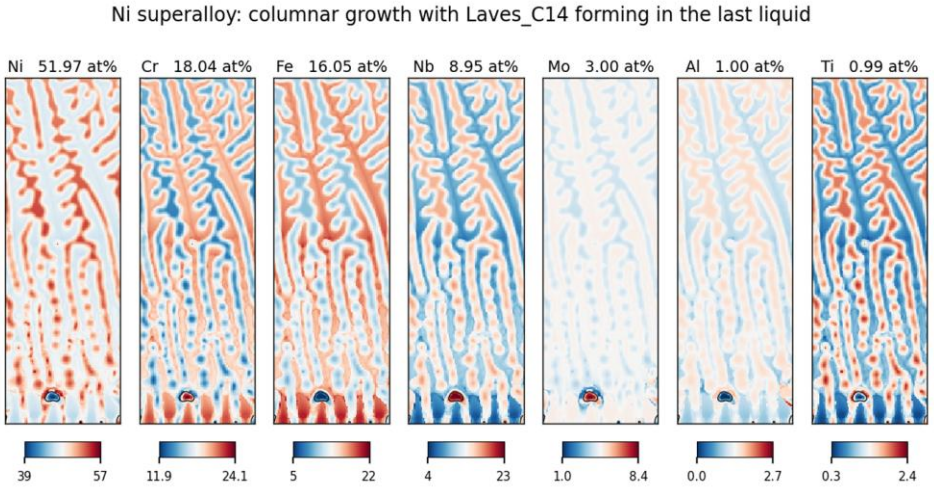

Fig. 3: OP Solidification Plugin: solidification of a Ni alloy (Ni-1Al-18Cr-16Fe-3Mo-9Nb-1Ti at%) under an 800 K/s cooling rate and a thermal gradient similar to additive manufacturing conditions. The microstructure shows the solute segregation associated with the formation of the primary Fcc phase and the Laves_C14 phase.

PandatAi and Pandat 2026A represent an important step toward the next generation of materials innovation, bringing together CALPHAD, ICME, and AI to make the materials design process simpler, smarter, and more efficient. We look forward to sharing PandatAi and Pandat 2026A with our users and collaborators.

References

[2009Bogno] Bogno, A., Nguyen-Thi, H., Billia, B., Bergeon, N., Mangelinck-Noël, N., Boller, E., … & Baruchel, J. (2009). In situ analysis of dendritic equiaxed microstructure formation in Al-Cu alloys by synchrotron X-ray radiography. *Transactions of the Indian Institute of Metals*, 62(4), 427-431.

[2017Tegeler] Tegeler, M., Shchyglo, O., Kamachali, R. D., Monas, A., Steinbach, I., & Sutmann, G. (2017). Parallel multiphase field simulations with OpenPhase. *Computer Physics Communications*, 215, 173-187.