



HEIDELBERG UNIVERSITY HOSPITAL







TOOLMAKER

LLM Agents Making Agent Tools



Georg Wölflein^{1,2,3,†}

Dyke Ferber^{3,4,‡}

Daniel Truhn⁵

Ognjen Arandjelović²

Jakob Nikolas Kather^{1,4,6}

¹EKFZ for Digital Health, TU Dresden ²University of St Andrews ⁴NCT, Heidelberg University Hospital ⁵University Hospital Aachen ⁶University Hospital Dresden

†work done while at EKFZ for Digital Health, TU Dresden and University of St Andrews

‡work done while at EKFZ for Digital Health, TU Dresden and NCT Heidelberg

Motivation

- LLM agents have predefined sets of tools
- Implementing new tools requires manual work & technical expertise



Employ agents to autonomously create new tools from research papers with code repositories

Components

Workflow state entails conversation history and environment state

$$s = (h, e) \in \mathcal{H} \times \mathcal{E}$$

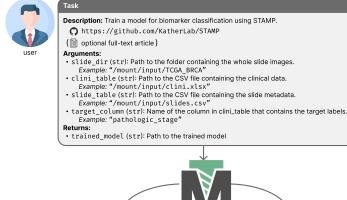
There are three types of workflow components (each act on state):

$$\frac{\mathcal{H} \times \mathcal{E}}{\text{old state}} \mapsto \frac{\mathcal{H} \times \mathcal{E}}{\text{new state}} \times \mathcal{R}$$

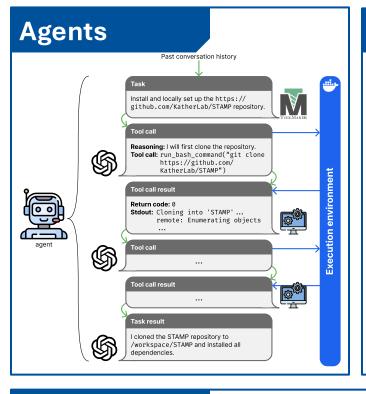
- **1. LLM calls** append to conversation history $\mathcal{H} \mapsto \mathcal{H} \times \mathcal{M}$
- 2. Environment interactions mutate environment state and return observation $\mathcal{E} \mapsto \mathcal{E} \times \mathcal{O}$ (O is the set of observations)
- 3. \boxtimes Agents do both: $\mathcal{H} \times \mathcal{E} \mapsto \mathcal{H} \times \mathcal{E} \times \mathcal{R}$

Problem

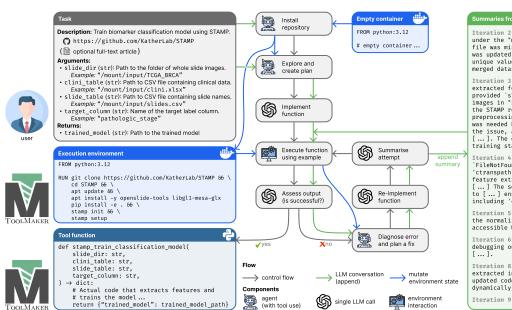
Given paper + GitHub repository + task **description**, generate an LLM-compatible tool







Workflow



Iteration 2: The configuration key `categories` under the 'modeling' section in the `config.yaml` file was missing [...] To fix this, the function was updated to infer the categories by extracting unique values from the `target_label` column of the merged dataset [...]

merged dataset [...]

Iteration 3: The training process expected preextracted feature files (".h5") [...] but the
provided 'slide dir' contained only raw slide
images in "svs" format. [...] Upon investigating
the STAMP repository, it was discovered that a
preprocessing step to extract features from slides
was needed before the actual training. [...] To fix
the issue, a preprocessing step was incorporated
[...]. The extracted features are passed to the
training stage [...]

Iteration 4: The [...] function failed with a 'FileNotFoundError' due to the absence of the 'ctranspath.pth' file [...] which was required for feature extraction using the 'preprocess' function. [...] The solution involved modifying the function to [...] ensure that all required model files, including 'ctranspath.pth', are downloaded [...]. Iteration 5: [\dots] A check was added to download the normalization template from the publicly accessible URL [\dots].

Iteration 8: [...] the `.h5` feature files were extracted into a deeper subdirectory [...]. In the updated code, after feature extraction, I dynamically resolved the correct subdirectory [...]

Main results

			TOOLMAKER (ours)				OpenHands (Wang et al., 2024)				
	Task	Invoc.	Tests	Cost	Actions	Tokens	Invoc.	Tests	Cost	Actions	Tokens
Pathology	conch_extract_features (Lu et al., 2024b)	3/3	9/9	\$0.35	15 (1 ₀)	171,226	3/3	9/9	\$0.08	5	51,701
	musk_extract_features (Xiang et al., 2025)	3/3	6/6	\$1.19	29 (6 ₀)	696,386	X	X	\$0.15	7	97,386
	pathfinder_verify_biomarker (Liang et al., 2023)	0/2	4/6	\$0.61	27 (1 ₀)	356,825	0/2	4/6	\$0.08	6	49,414
	stamp_extract_features (El Nahhas et al., 2024)	3/3	12/12	\$1.12	20 (4 ₀)	631,138	0/3	3/12	\$0.07	6	42,793
	stamp_train_classification_model (El Nahhas et al., 2024)	3/3	9/9	\$2.27	33 (9 ₀)	1,249,521	0/3	0/9	\$0.15	8	87,915
	uni_extract_features (Chen et al., 2024)	3/3	9/9	\$0.61	16 (4 ₀)	326,806	X	X	\$0.25	10	177,119
Radiology	medsam_inference (Ma et al., 2024)	3/3	6/6	\$0.96	18 (6 ₀)	508,954	X	Х	\$0.07	5	41,096
	nnunet_train_model (Isensee et al., 2020)	0/2	0/4	\$2.90	35 (9 ₀)	1,792,291	0/2	0/4	\$0.12	8	79,231
Omics	cytopus_db (Kunes et al., 2023)	3/3	12/12	\$0.41	10 (3 ₀)	185,912	X	X	\$0.36	8	236,217
	esm_fold_predict (Verkuil et al., 2022; Hie et al., 2022)	2/3	13/15	\$0.66	20 (1 ₀)	336,754	X	X	\$0.11	6	69,493
Other	flowmap_overfit_scene (Smith et al., 2024)	2/2	6/6	\$0.70	18 (5 ₀)	358,552	X	X	\$0.36	15	250,787
	medsss_generate (Jiang et al., 2025)	3/3	6/6	\$0.53	25 (3 ₀)	282,771	3/3	6/6	\$0.15	10	104,505
	modernbert_predict_masked (Warner et al., 2024)	3/3	9/9	\$0.66	20 (4 ₀)	356,228	X	X	\$0.13	10	82,930
	retfound_feature_vector (Zhou et al., 2023)	3/3	6/6	\$0.97	31 (5 ₀)	561,936	0/3	0/6	\$0.08	4	46,521
	tabpfn_predict (Hollmann et al., 2025)	3/3	9/9	\$0.23	10 (1 ₀)	95,257	3/3	9/9	\$0.07	4	36,320

Conclusion

Autonomous tool creation is feasible for complex scientific tasks

