ToolMaker

LLM Agents Making Agent Tools

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Motivation

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

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

Components

Workflow **state** entails **conversation history** and **environment state**

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

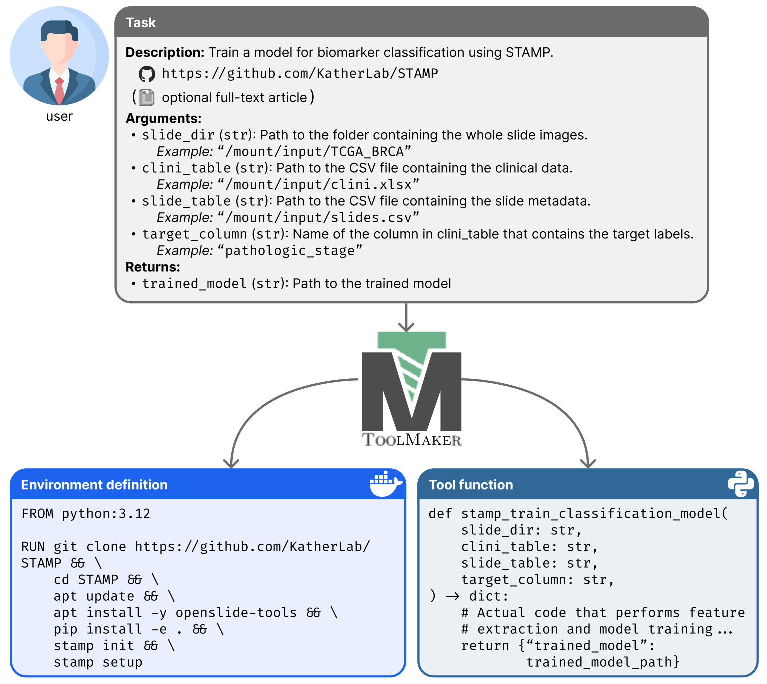
There are three types of workflow components (each act on state):

$$\underbrace{\mathcal{H}\times\mathcal{E}}_{\text{old state}} \mapsto \underbrace{\mathcal{H}\times\mathcal{E}}_{\text{new state}}\times\underbrace{\mathcal{R}}_{\text{return value}}$$

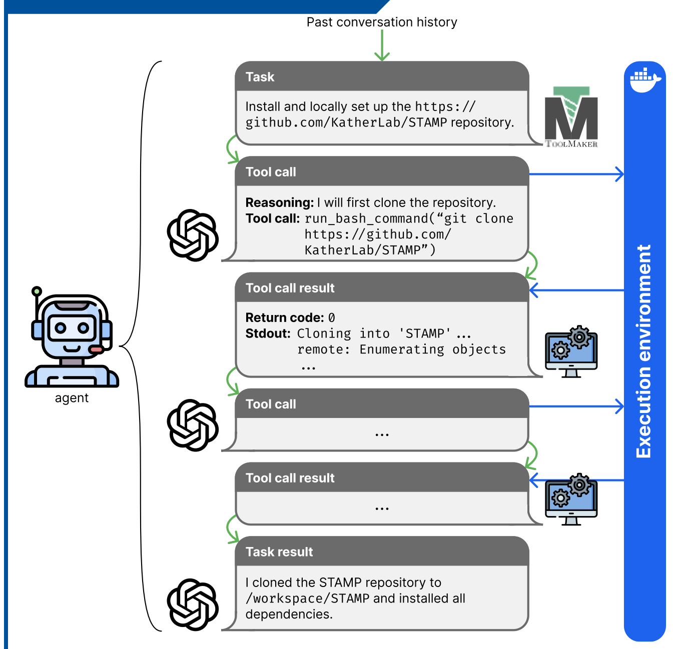
1. **LLM calls** append to conversation history $\mathcal{H} \mapsto \mathcal{H} \times \mathcal{M}$
2. **Environment interactions** mutate environment state and return observation $\mathcal{E} \mapsto \mathcal{E} \times \mathcal{O}$ ($\mathcal{O}$ is the set of observations)
3. **Agents** do both: $\mathcal{H}\times\mathcal{E}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

Problem

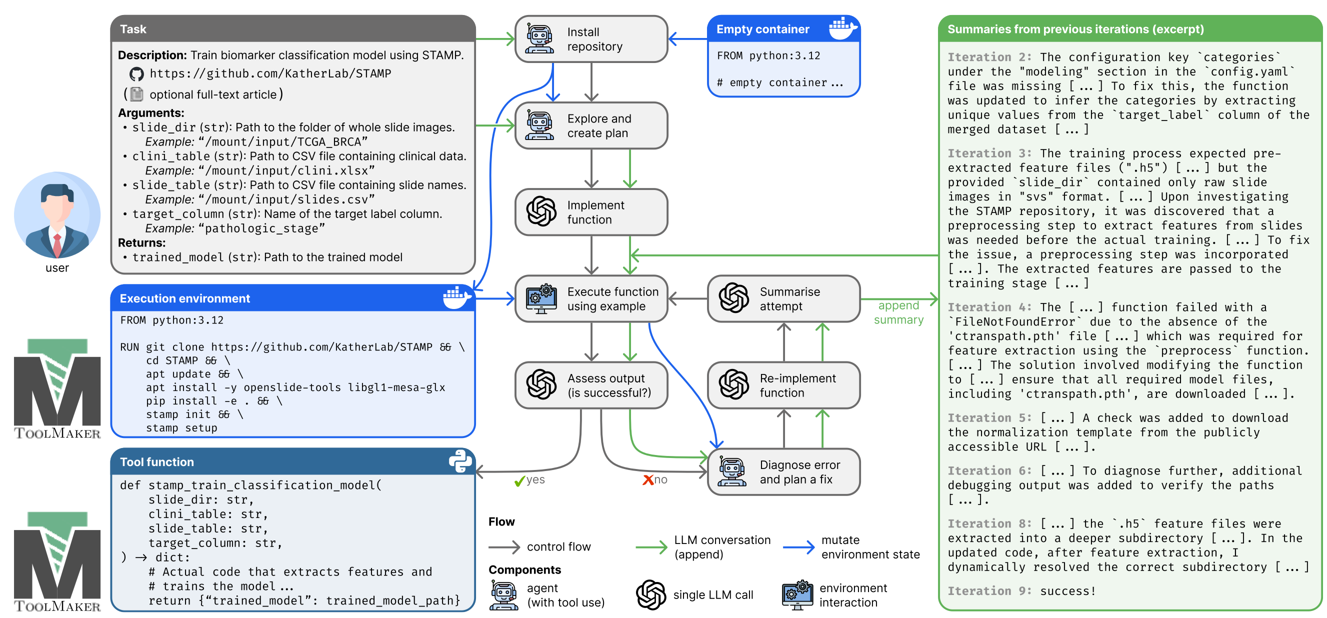
Given **paper** + GitHub **repository** + task **description**, generate an LLM-compatible tool



Agents



Workflow



Main results

	Task	ToolMaker (ours) Invoc.	Tests	Cost	Actions	Tokens	OpenHands (Wang et al., 2024) Invoc.	Tests	Cost	Actions	Tokens
Pathology	conch_extract_features (Lu et al., 2024b)	3/3	9/9	\$0.35	15 ($1_{\circlearrowleft}$)	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 ($6_{\circlearrowleft}$)	696,386	✗	✗	\$0.15	7	97,386
	pathfinder_verify_biomarker (Liang et al., 2023)	0/2	4/6	\$0.61	27 ($1_{\circlearrowleft}$)	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 ($4_{\circlearrowleft}$)	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 ($9_{\circlearrowleft}$)	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 ($4_{\circlearrowleft}$)	326,806	✗	✗	\$0.25	10	177,119
Radiology	medsam_inference (Ma et al., 2024)	3/3	6/6	\$0.96	18 ($6_{\circlearrowleft}$)	508,954	✗	✗	\$0.07	5	41,096
	nnunet_train_model (Isensee et al., 2020)	0/2	0/4	\$2.90	35 ($9_{\circlearrowleft}$)	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 ($3_{\circlearrowleft}$)	185,912	✗	✗	\$0.36	8	236,217
	esm_fold_predict (Verkuil et al., 2022; Hie et al., 2022)	2/3	13/15	\$0.66	20 ($1_{\circlearrowleft}$)	336,754	✗	✗	\$0.11	6	69,493
Other	flowmap_overfit_scene (Smith et al., 2024)	2/2	6/6	\$0.70	18 ($5_{\circlearrowleft}$)	358,552	✗	✗	\$0.36	15	250,787
	medsss_generate (Jiang et al., 2025)	3/3	6/6	\$0.53	25 ($3_{\circlearrowleft}$)	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 ($4_{\circlearrowleft}$)	356,228	✗	✗	\$0.13	10	82,930
	retfound_feature_vector (Zhou et al., 2023)	3/3	6/6	\$0.97	31 ($5_{\circlearrowleft}$)	561,936	0/3	0/6	\$0.08	4	46,521
	tabpfn_predict (Hollmann et al., 2025)	3/3	9/9	\$0.23	10 ($1_{\circlearrowleft}$)	95,257	3/3	9/9	\$0.07	4	36,320

Conclusion

Autonomous tool creation is feasible for complex scientific tasks