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From Traditional Scientists to Agentic AI Research: Unequivocal Diagram-as-Code in Scientific Publications

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Method Article

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From Traditional Scientists to Agentic AI Research: Unequivocal Diagram-as-Code in Scientific Publications

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Abstract

Background

Textual descriptions and visual representations both offer substantial space for varied interpretations. One of the enduring goals of artificial intelligence (AI) development is to create systems capable of making scientific discoveries autonomously.

Results

This work proposes the use of diagrams-as-code in scientific papers to ensure that published information can be unequivocally interpreted by scientists, large language models (LLMs), and AI systems that rely on LLMs. Simultaneously, this approach would facilitate reliable handoffs between scientific literature and scientists, scientific literature and AI agents, and among AI agents within research pipelines. Furthermore, the proposed approach can, unrelated to scientific

publications, enable consistent transfers when processes are subjects of AI agents' handoffs, independent of scientific publications.

Conclusion

The viability of this approach is demonstrated through three representative examples of scientific textual descriptions and visual representations, along with their corresponding diagrams-as-code.

Keywords: scientific publication, biomedical literature, AI agent, agentic AI, diagram-as-code

Background

Natural languages have established methods for producing a limitless variety of linguistic expressions. However, they also inherently allow for significant interpretative variability—the meaning assigned to a specific utterance can differ widely, influenced by factors such as the speaker's background, the context in which it occurs, and the preceding discourse [1].

Nature is highly complex. To study its principles, scientists isolate specific phenomena and examine their features through visual models and representations [2,3]. These models enable investigations to be conducted directly on such representations rather than on reality itself [3]. Visual representations aid in replicating reality while also assisting in solving problems and filling gaps in knowledge [4]. Diagrams can be combined, rearranged, and superimposed in various ways, allowing concepts from different sources to be studied simultaneously, revealing new connections and elements of the phenomena [5]. Additionally, visual representation is a crucial aspect of academic articles, used to convey scientific information and support conceptual understanding of the presented content [4]. Schematic illustrations are widely employed in academic papers, posters, and conferences to communicate complex scientific concepts. Well-structured illustrations often offer significant advantages over textual descriptions, as they can provide a more intuitive and

concise means of conveying novel discoveries and facilitating effective scientific knowledge exchange [6]. However, interpretations of visual representations can also differ among individuals due to prior knowledge, assumptions about what the visual represents, and individual object features like size, shape, and contrast [7].

One of the enduring goals of AI development is to create systems that can make scientific discoveries. It is anticipated that AI agents will soon help streamline scientific research workflows, making them faster and more resource-efficient. This advancement would support continuous, high-throughput research at a scale and pace that would be unfeasible for human researchers to achieve independently [8]. Research pipelines are increasingly incorporating agentic AI systems to automate complex, multi-step knowledge compilation processes [9]. Throughout its development trajectory, AI has evolved from standalone LLMs to more autonomous, task-oriented systems. This progress has unfolded in several phases. Initially, generative agents emerged, implemented with LLMs, designed to generate novel outputs such as text, code, and images based on user prompts. Subsequently, a new class of systems—AI agents—was developed. These agents augment LLMs with the ability to interact with external tools, invoke functions, and perform sequential reasoning, thereby enabling the autonomous retrieval of real-time information and execution of complex, multi-step workflows. AI has advanced further into agentic AI, composed of multiple specialized agents that coordinate and cooperate to achieve common goals. Unlike general-purpose LLMs, agents are characterized by structured initialization, bounded autonomy, and sustained focus on specific tasks. Although generative agents, AI agents, and agentic AI employ different interaction models and levels of autonomy, they all rely on LLMs as their core reasoning engines [9].

LLMs capture extensive statistical and semantic patterns, enabling them to perform tasks such as inference, summarization, code generation, and dialogue management. However, within agentic systems, LLMs serve purposes beyond response generation. They function as cognitive engines

that interpret user objectives, assess potential action plans, select appropriate strategies, use external tools, and coordinate complex, multi-step workflows [9].

AI agents built on LLMs are subject to various intrinsic limitations inherited from the underlying language models. One of the most significant limitations is their tendency to generate hallucinations—outputs that appear plausible but are factually incorrect. Moreover, even slight changes in prompt wording can yield substantially different outputs. These limitations reduce the consistency and reproducibility of LLM outputs. Furthermore, errors can be amplified when inaccurate or hallucinated output from one agent propagates through an AI agent-based system, resulting in larger inaccuracies and compromising subsequent decisions [9].

This work proposes a new approach for representing information in scientific literature to promote standardized and unequivocal interpretation by scientists, LLMs, and AI systems that rely on LLMs. Additionally, the proposed approach would enable reliable handoffs between scientific literature and scientists, between scientific literature and AI agents, and among AI agents in research pipelines. Furthermore, the proposed approach can ensure that processes subject to AI-agent handoffs are transferred consistently.

Methods

Three typical examples of textual descriptions and visual representations were used as input to generate diagrams-as-code. They were formatted and presented as they typically appear in scientific literature.

The following three text snippets were used as typical examples of textual descriptions:

1. “Regardless of the initiating clinical cause—ischemic injury, pressure overload, volume overload, cardiomyopathy, myocarditis, arrhythmia, metabolic disease or valvular pathology—the failing heart is characterized by persistent activation of neurohormonal, mechanical, inflammatory,

oxidative and metabolic signaling pathways. These pathways initially preserve cardiac output, but chronic stimulation progressively alters cardiomyocyte phenotype, fibroblast activity, vascular function, mitochondrial metabolism and intercellular communication."

2. "Heart failure is not a single disease but a clinical syndrome that develops when structural or functional abnormalities of the heart impair ventricular filling, ventricular ejection, or both. The initial insult may be ischemic myocardial injury, chronic pressure overload from hypertension or aortic stenosis, volume overload from valvular regurgitation, primary cardiomyopathy, myocarditis, tachyarrhythmia, congenital heart disease, toxic injury, infiltrative disease, or a combination of cardiovascular and systemic risk factors such as diabetes, chronic kidney disease, obesity, anemia, and chronic inflammation."

3. "In a stable patient with suspected chronic heart failure, the pathway usually starts at primary care or general internal medicine level. The first visit should include a detailed history, medication review, assessment of cardiovascular risk factors, previous cardiac disease, alcohol and toxin exposure, cancer therapy, family history, and precipitating conditions such as infection, anemia, renal deterioration, uncontrolled hypertension, atrial fibrillation, ischemia, pulmonary embolism, thyroid disease, non-adherence to medication, excess salt intake, or use of drugs that worsen fluid retention. Physical examination should assess blood pressure, heart rate and rhythm, oxygen saturation, body weight, jugular venous pressure, lung crackles, pleural effusion, displaced apex beat, murmurs, hepatomegaly, ascites, peripheral edema, peripheral perfusion, and signs of frailty."

Examples of typical visual representations used as inputs are provided in Figures 1–3.

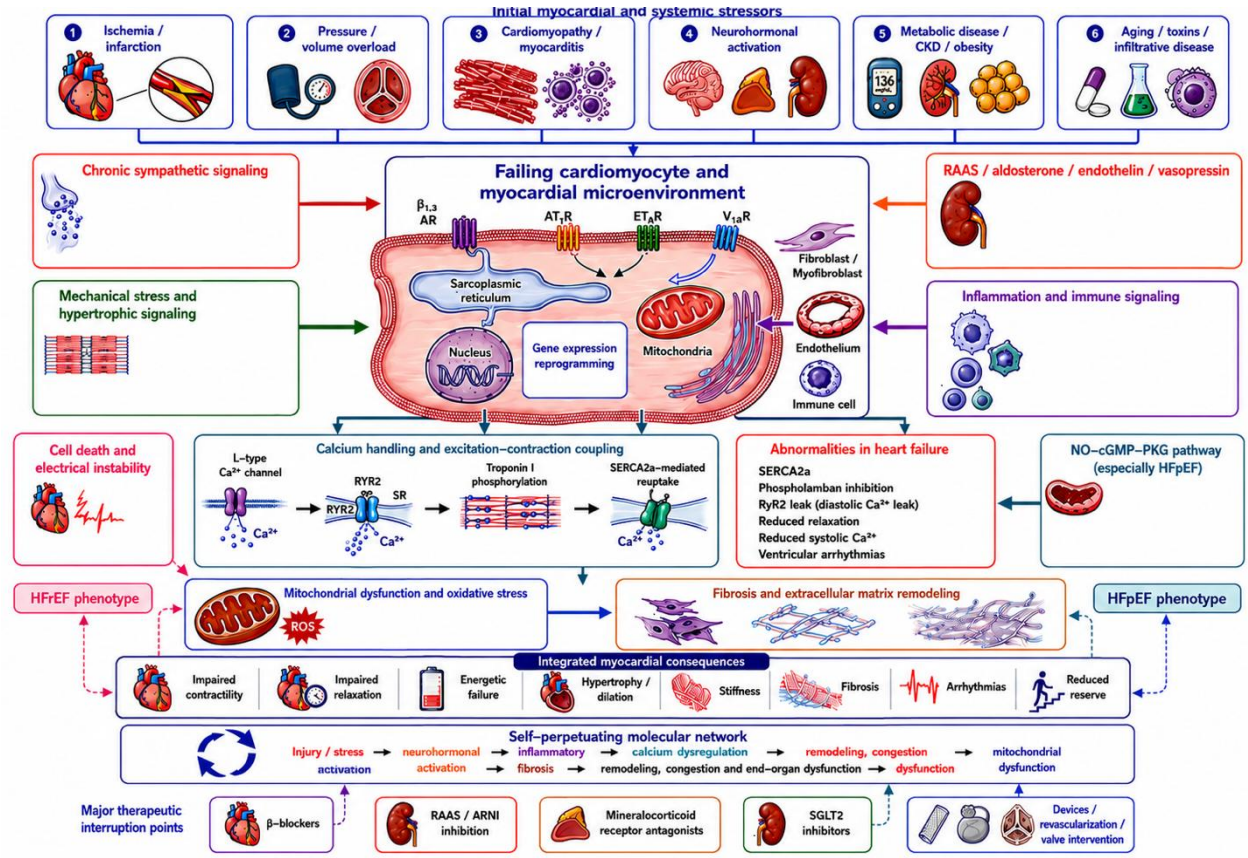


Figure 1. Molecular, biochemical and signaling mechanisms in heart failure

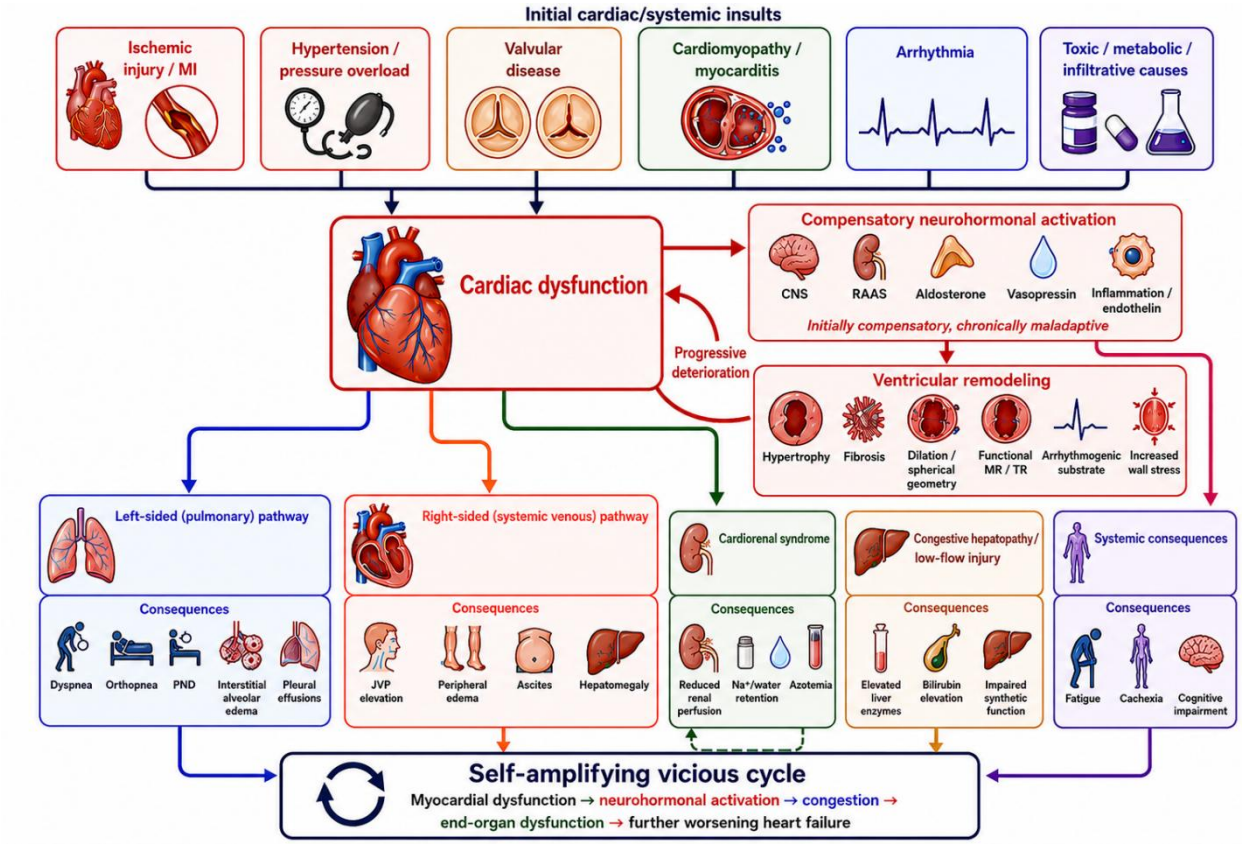


Figure 2. Pathophysiological cascade of heart failure

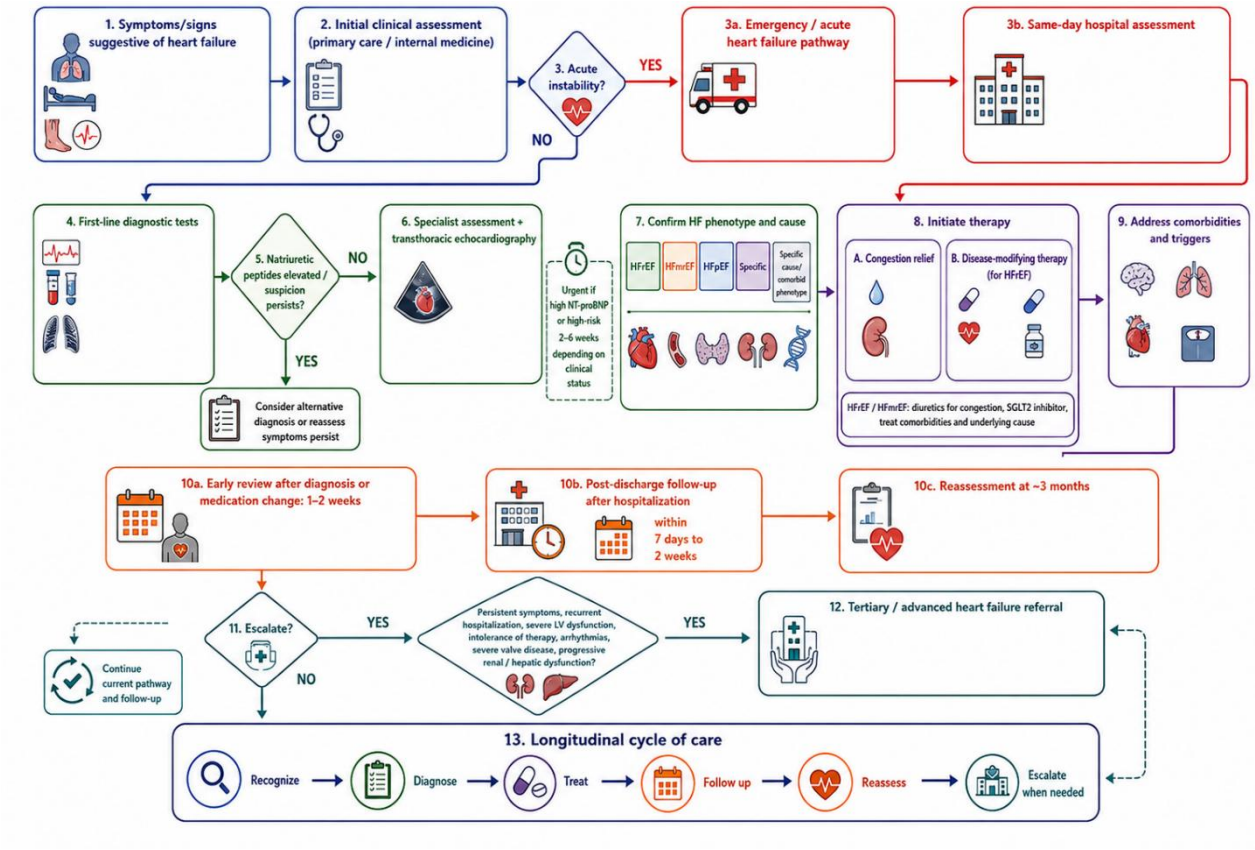


Figure 3. Clinical pathway for suspected and confirmed heart failure

The ChatGPT (https://chatgpt.com) free plan was used during the period from July 4 to 15, 2026 to create diagrams-as-code. Code for one Mermaid diagram and one D2 diagram was generated for each typical example of a textual description and visual representation.

To generate code for Mermaid diagrams from textual descriptions, the following prompt was used for each of the three descriptions: “Create code for a Mermaid diagram for this.” For code generation for D2 diagrams, the following prompt was used: “Create code for a D2 diagram for this.”

To generate code for Mermaid diagrams from figures, the following prompt was used for each of the three figures: “Create code for a Mermaid diagram for this figure. Do not add anything

yourself." For code generation for D2 diagrams, the following prompt was used: "Create code for a D2 diagram for this figure. Do not add anything yourself."

Mermaid diagrams were visually verified using the Mermaid Live Editor (https://mermaid.live/edit), and D2 diagrams were verified in the D2 Playground (https://play.d2lang.com/). Some minor edits were made afterward to some of the diagrams-as-code to reflect the intended representation (e.g., adjustments to the direction of some arrows and the replacement of element-to-element links within blocks with block-to-block links).

Results

Textual descriptions to diagrams-as-code

For all three textual descriptions, which define processes at different levels and across various subdomains, representative diagrams-as-code were generated, demonstrating the feasibility of the proposed approach.

For text 1, which discusses shared pathophysiological mechanisms of heart failure, code for a Mermaid diagram (Additional file 1) and D2 diagram (Additional file 2) were generated and visually verified in the corresponding editors (Figure 4).

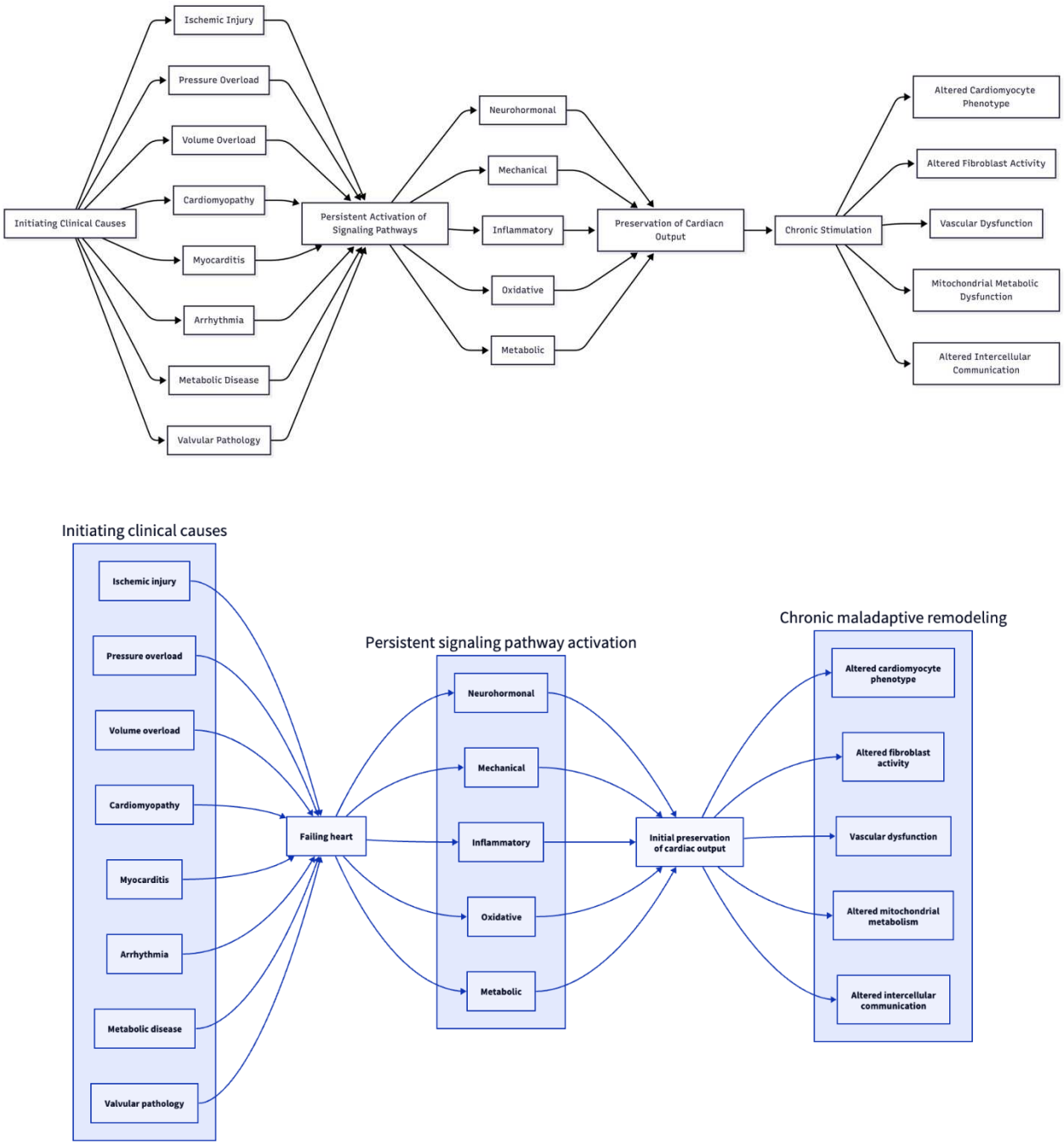


Figure 4. Shared pathophysiological mechanisms of heart failure—Mermaid diagram (top) and D2 diagram (bottom)

For text 2, which defines and describes the etiology of heart failure, code for a Mermaid diagram (Additional file 3) and a D2 diagram (Additional file 4) were generated and visually verified in the corresponding editors (Figure 5).

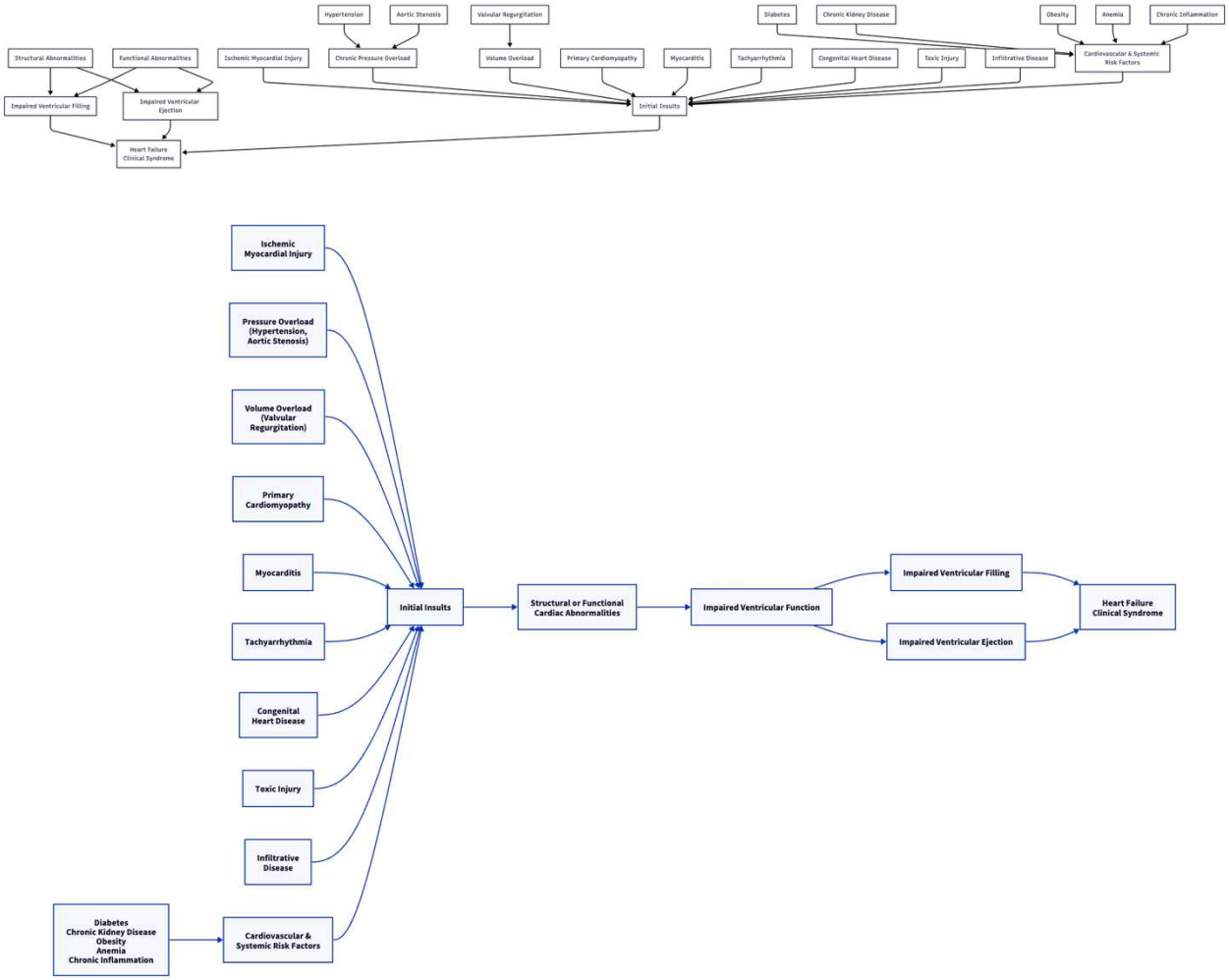


Figure 5. Definition and etiology of heart failure—Mermaid diagram (top) and D2 diagram (bottom)

For text 3, which addresses the initial evaluation of stable patients with suspected chronic heart failure, code for a Mermaid diagram (Additional file 5) and a D2 diagram (Additional file 6) were generated and visually verified in the corresponding editors (Figure 6).

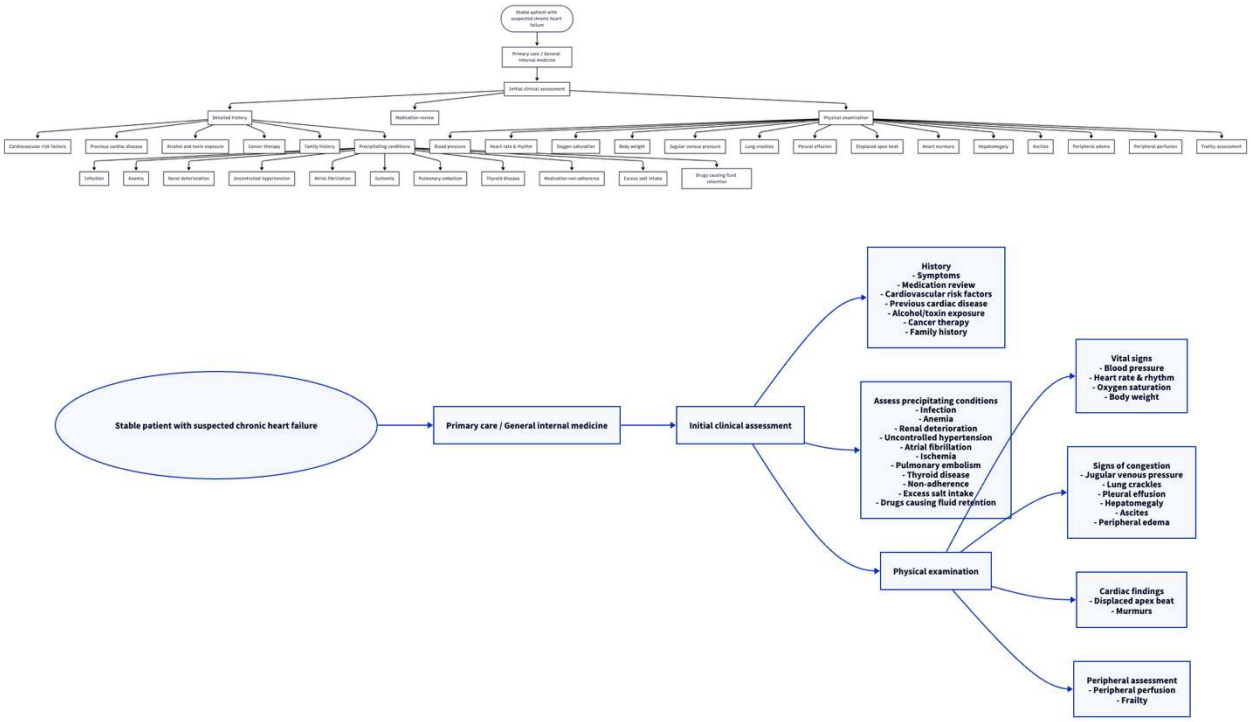


Figure 6. Initial evaluation of stable patients with suspected chronic heart failure—Mermaid diagram (top) and D2 diagram (bottom)

Figures to diagrams-as-code

For all three figures used (Figures 1–3), which illustrate processes at different levels and across various subdomains, representative diagrams-as-code were generated, demonstrating the feasibility of the proposed approach.

For the Figure 1, which depicts molecular, biochemical, and signaling mechanisms in heart failure, code for a Mermaid diagram (Additional file 7) and a D2 diagram (Additional file 8) were generated and visually verified in the corresponding editors (Figure 7).

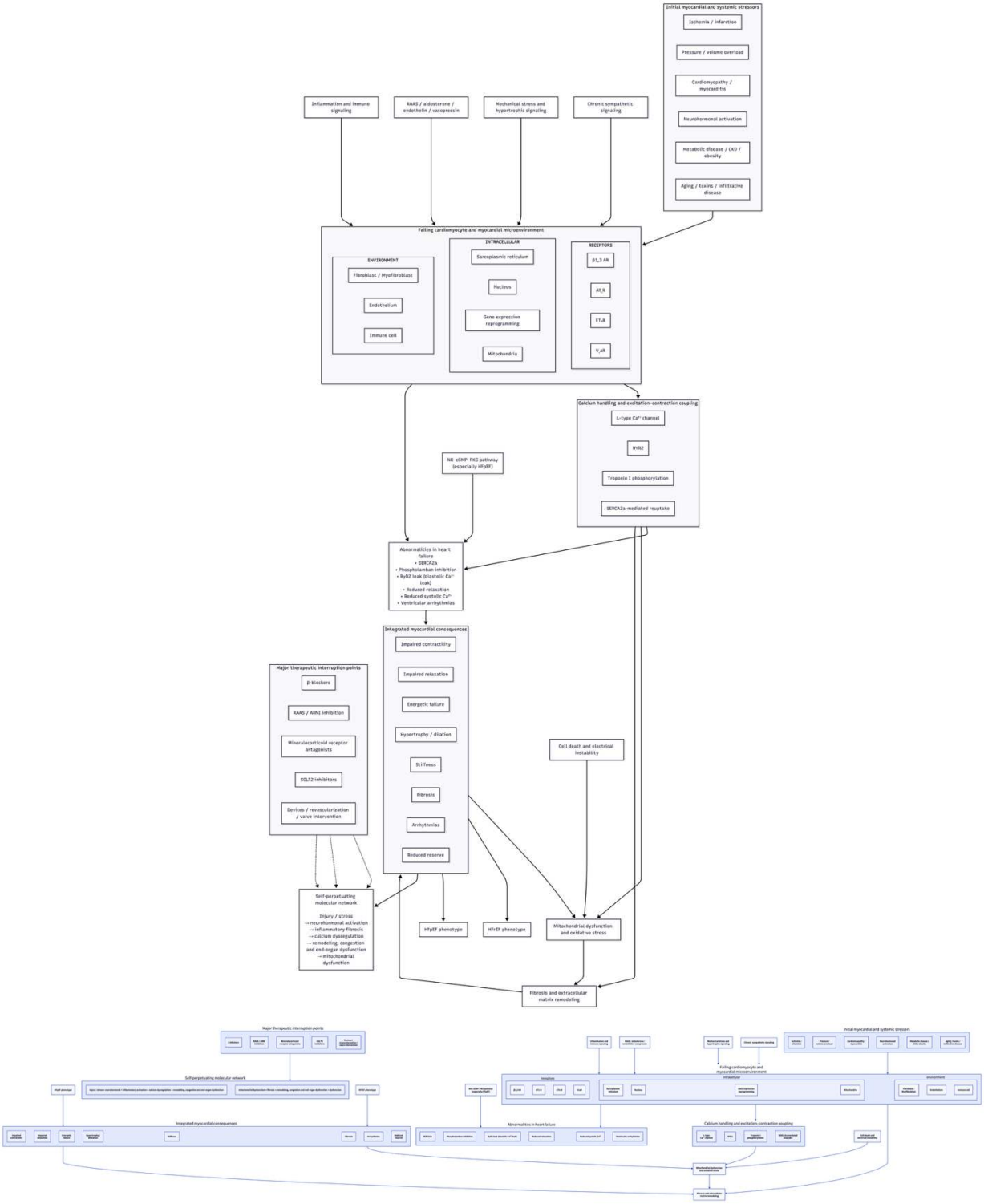


Figure 7. Molecular, biochemical, and signaling mechanisms in heart failure—Mermaid diagram (top) and D2 diagram (bottom)

For the Figure 2, which illustrates the pathophysiological cascade of heart failure, code for a Mermaid diagram (Additional file 9) and a D2 diagram (Additional file 10) diagram were generated and visually verified in the corresponding editors (Figure 8).

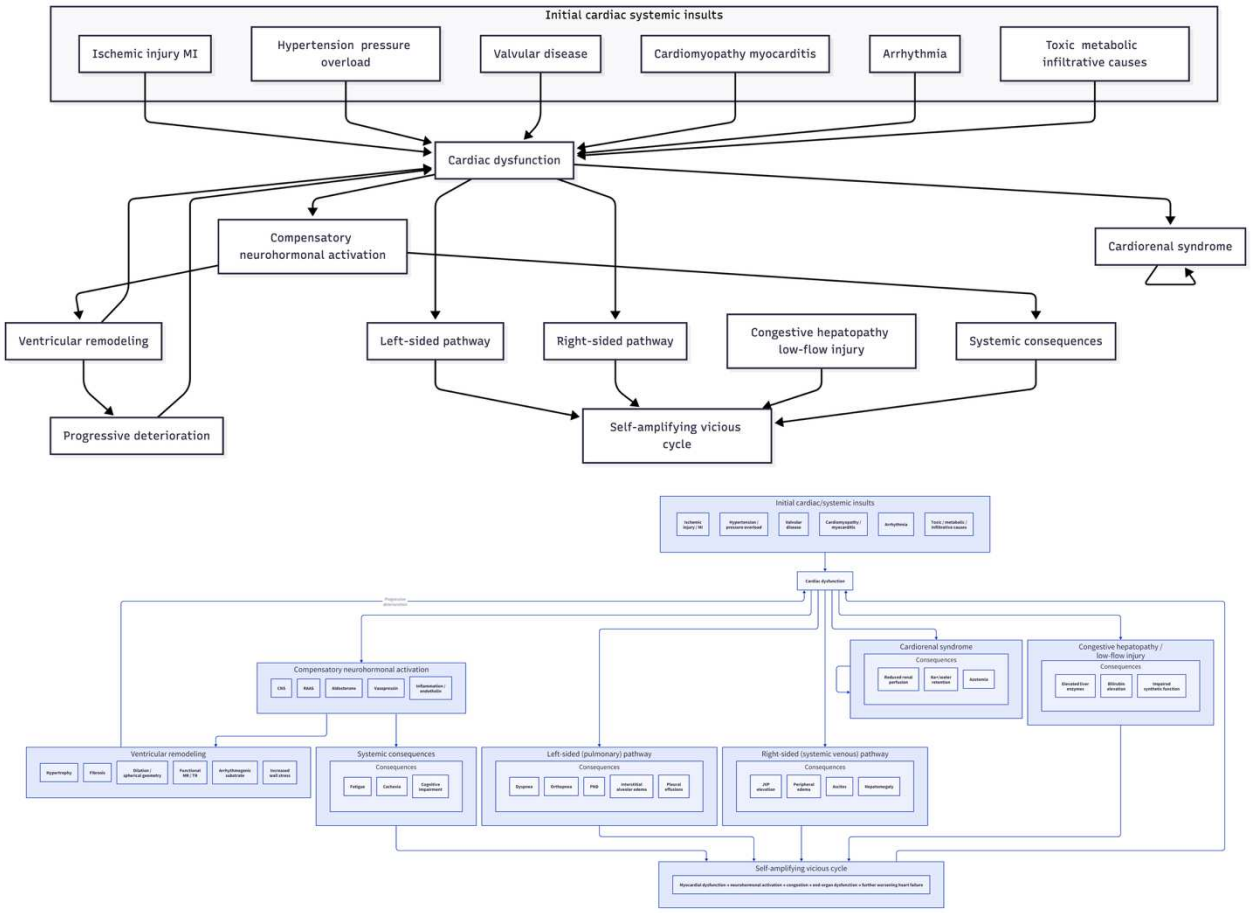


Figure 8. Pathophysiological cascade of heart failure—Mermaid diagram (top) and D2 diagram (bottom)

For Figure 3, which outlines the clinical pathway for suspected and confirmed heart failure, code for a Mermaid diagram (Additional file 11) and a D2 diagram (Additional file 12) were generated and visually verified in the corresponding editors (Figure 9).

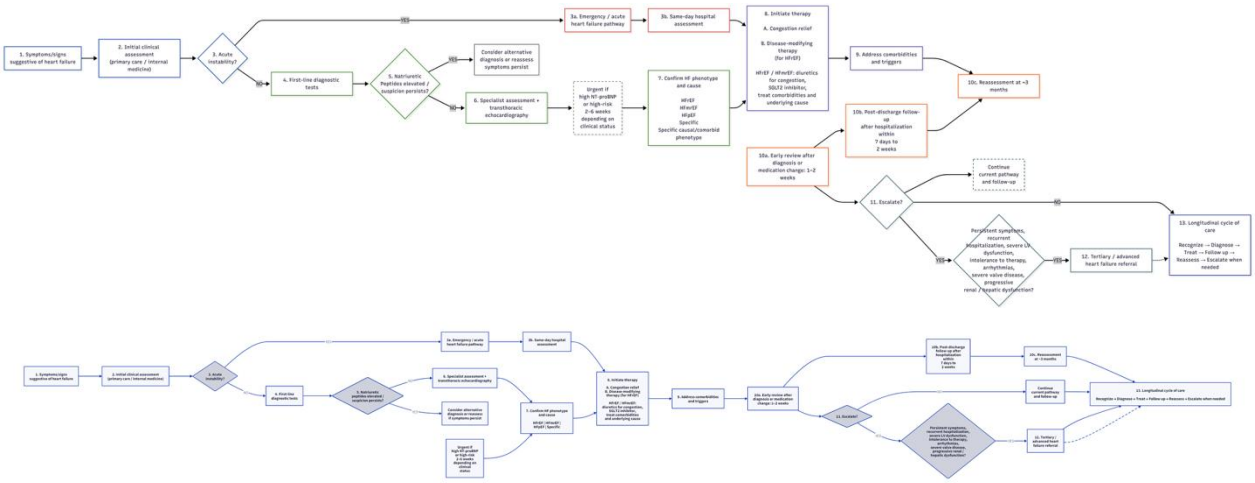


Figure 9. Clinical pathway for suspected and confirmed heart failure—Mermaid diagram (top) and D2 diagram (bottom)

Discussion

In this paper, we present and propose diagram-as-code as a consistent alternative to the three typical examples of textual descriptions and visual representations in scientific literature. We advocate for information codification to minimize or eliminate interpretative variability. The same textual description and visual representation can be interpreted differently by scientists and LLMs. Although standardized representations exist in some scientific fields (e.g., chemical formulas in chemistry), there is currently no widely adopted method for representing processes across scientific literature, despite their frequent depiction as unstandardized diagrams in publications.

Generating simple code snippets has become accessible to everyone due to the availability of LLM chat interfaces. In our proposed approach, such generated code can be rendered in available editors, allowing users to verify that the process has been represented correctly. Diagram-as-code syntax is designed to be intuitive and easily comprehensible. If necessary, modifications can be made using LLMs or by manually editing the code.

We demonstrated the approach using Mermaid and D2 diagrams, but other tools and software that support diagrams-as-code and provide public editors, such as PlantUML (https://plantuml.com) and Graphviz (https://graphviz.org), could also be used. Some of these tools even have AI capabilities for further diagram refinement through interaction with the tool. Additionally, other LLMs and LLM chat interfaces can be employed for generating diagrams-as-code, based on user preferences.

It is important to emphasize that the code serves as the unit that captures unequivocal representation, while the diagram is merely a visual way to confirm that the intended meaning is preserved during code generation. Some LLM chat interfaces even display Mermaid diagrams for the code they generate as part of their responses.

Some publications from various disciplines (glaciology, giftedness and talent development, and programming languages) have already employed Mermaid diagrams [10-12], and the source code for these diagrams unequivocally represents the processes depicted.

We propose that diagrams-as-code be integrated into existing scientific literature formats to codify and unequivocally state the most important points. The approach proposed in this paper makes handoffs between textual/visual representations and scientists, between textual/visual representations and AI, as well as among AI agents deterministic and consistent. In the context of agentic AI, when a new AI agent takes over further work on a process that is the subject of research, it can verify whether the process representation still aligns with the original or corresponding upstream version and proceed only if it does. A similar process is possible for any other handoff of such representations in research or scientific publishing.

Limitations

Known elements and their relationships can be codified; however, for many processes, some elements and relationships remain unknown and cannot be represented. Nevertheless, this limitation pertains more to the current state of knowledge than to the proposed approach itself.

If diagrams are created with the assistance of LLMs, hallucinations in the diagrams are possible. However, this limitation underscores the importance of the proposed verification step, in which the diagram is confirmed to reflect the intended representation in the editor.

Although more sophisticated prompt engineering can be applied, we intentionally used the simplest prompts to demonstrate that even with these, satisfactory results can be achieved.

Future research directions

The proposed approach can be further improved by providing recommendations on the best tools and coding languages for specific scientific contexts, or by creating new tools and coding languages that could support standardized overarching scientific representation.

Current knowledge is also represented in knowledge graphs, some of which are publicly available. The integration of the proposed approach with knowledge graphs and the potential applications of this integration could be explored further.

Conclusion

We propose the use of diagrams-as-code in scientific papers as an approach that can bring standardization to scientific textual descriptions and visual representations, ensuring unequivocal interpretation of the represented processes by scientists, LLMs, and AI systems relying on LLMs. The feasibility of the proposed approach has been demonstrated through three representative

examples of scientific textual descriptions and visual representations, along with their corresponding generated diagrams-as-code.

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Availability of data and materials

All data generated or analyzed during this study are included in this published article (and its supplementary information files).

Code Availability

All code generated or analyzed during this study is included in this published article (and its supplementary information files).

Competing Interest Declaration

The authors declare no competing interests.

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Authors' contributions

MG and LV substantially contributed to the conception and design of the work, analysis and interpretation of data, drafted and revised the work, and approved the submitted version. All authors read and approved the final manuscript.

Acknowledgements

Not applicable

Ethics

Not applicable

Consent to Participate

Not applicable

Consent to Publish

Not applicable

Additional files

Additional file 1.txt Code for a Mermaid diagram generated for text 1

Additional file 2.txt Code for D2 diagram generated for text 1

Additional file 3.txt Code for a Mermaid diagram generated for text 2

Additional file 4.txt Code for D2 diagram generated for text 2

Additional file 5.txt Code for a Mermaid diagram generated for text 3

Additional file 6.txt Code for D2 diagram generated for text 3

Additional file 7.txt Code for a Mermaid diagram generated for Figure 1

Additional file 8.txt Code for D2 diagram generated for Figure 1

Additional file 9.txt Code for a Mermaid diagram generated for Figure 2

Additional file 10.txt Code for D2 diagram generated for Figure 2

Additional file 11.txt Code for a Mermaid diagram generated for Figure 3

Additional file 12.txt Code for D2 diagram generated for Figure 3

Supplementary Files

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