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The MICROCARD project

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► **To cite this version:**

Mark Potse. The MICROCARD project. EuroHPC Summit 2024 - The European High Performance Computing, Mar 2024, Antwerp, Belgium. hal-04713117

HAL Id: hal-04713117

<https://inria.hal.science/hal-04713117v1>

Submitted on 30 Sep 2024

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The MICROCARD project

This poster was authored for the MICROCARD consortium by Mark Potse (IHU Liryc, Bordeaux, France; CARMEN team, Inria, France; and Institut de mathématiques de Bordeaux, UMR5251, Talence, France) for presentation at the 2024 EuroHPC Summit meeting which took place from 18 to 21 March 2024 in Antwerp, Belgium.

This project has received funding from the European High-Performance Computing Joint Undertaking EuroHPC (JU) under grant agreement No 955495. The JU receives support from the European Union's Horizon 2020 research and innovation programme and France, Italy, Germany, Austria, Norway, and Switzerland. The project was co-funded by the French National Research Agency ANR, the German Federal Ministry of Education and Research, the Italian ministry of economic development, the Swiss State Secretariat for Education, Research and Innovation, the Austrian Research Promotion Agency FFG, and the Research Council of Norway.

The MICROCARD project

Modeling the heart cell by cell on exascale supercomputers

The contraction of the heart is coordinated electrically thanks to conducting links between the cells. Structural damage, due to aging or disease, can break these links and cause dangerous arrhythmia.

To better understand these arrhythmia we need models in which the individual cells and their connections are resolved. For a whole heart, with billions of cells, this means trillions of model elements with many degrees of freedom each.

The MICROCARD project aims to run such models on exascale computers. It covers every aspect of this challenge from code transformations to numerical schemes, mesh creation, and real-life use cases.

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Cardiac electrical activity can be modeled with a large **reaction-diffusion** system. Traditionally this is done with a homogenization approach so that model elements average the behaviour of hundreds of cells. **The goal of MICROCARD is to discretize individual cells and their interconnections.**

The **reaction term** represents the currents generated by ion channels and pumps everywhere in the cell membrane. It is governed by a system of ordinary differential equations with strongly nonlinear coefficients.

$$\begin{aligned}
 J_{Ca} &= G_{Ca} m^2 h_j (V_m - E_{Ca}) \\
 J_{K1} &= (m_{\infty} - m) / \tau_m \\
 J_{K2} &= (n_{\infty} - n) / \tau_n \\
 J_{K3} &= (j_{\infty} - j) / \tau_j \\
 m_{\infty} &= [1 + \exp(-56.86 - V_m) / 9.03]^{-1} \\
 \tau_m &= \alpha_m V_m \\
 n_{\infty} &= [1 + \exp(-60 - V_m) / 5]^{-1} \\
 \tau_n &= 0.1 / [1 + \exp(V_m + 35 / 5)] \\
 j_{\infty} &= 0.1 / [1 + \exp(V_m + 50 / 200)] \\
 h_{\infty} &= [1 + \exp(V_m + 71.53 / 7.43)]^{-1} \\
 \tau_h &= (\alpha_h h_j)^{-1} \\
 \alpha_h &= \begin{cases} 0 & \text{if } V \geq -40\text{mV} \\ 0.057 \exp(-V_m + 80) / 6.8 & \text{otherwise} \end{cases} \\
 &\text{(10 more lines like that)}
 \end{aligned}$$

The **diffusion term** is a large system of linear equations ($N \sim 10^{12}$)

In our cellular-scale model, an additional difficulty is that the reaction term is an internal boundary condition, as it is present in the membrane of every cell.

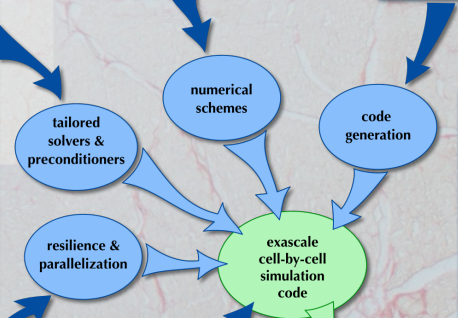
MLIR

Using models expressed in a domain-specific language and compiled using the multilevel intermediate representations (MLIR) framework, we can now compute membrane currents about 2 times faster on vector CPUs and many times faster on GPUs. The speedup is larger for more compute-intensive models.

Model	Nvidia A100 (GFLOPS)	AVX-512 (GFLOPS)	baseline (GFLOPS)
Abrahamson	10	10	10
Abrahamson+Katz	15	15	15
Abrahamson+Katz+Koch	20	20	20
Abrahamson+Katz+Koch+Koch	25	25	25
Abrahamson+Katz+Koch+Koch+Koch	30	30	30
Abrahamson+Katz+Koch+Koch+Koch+Koch	35	35	35
Abrahamson+Katz+Koch+Koch+Koch+Koch+Koch	40	40	40
Abrahamson+Katz+Koch+Koch+Koch+Koch+Koch+Koch	45	45	45
Abrahamson+Katz+Koch+Koch+Koch+Koch+Koch+Koch+Koch	50	50	50
Abrahamson+Katz+Koch+Koch+Koch+Koch+Koch+Koch+Koch+Koch	55	55	55
Abrahamson+Katz+Koch+Koch+Koch+Koch+Koch+Koch+Koch+Koch+Koch	60	60	60
Abrahamson+Katz+Koch+Koch+Koch+Koch+Koch+Koch+Koch+Koch+Koch+Koch	65	65	65
Abrahamson+Katz+Koch+Koch+Koch+Koch+Koch+Koch+Koch+Koch+Koch+Koch+Koch	70	70	70
Abrahamson+Katz+Koch+Koch+Koch+Koch+Koch+Koch+Koch+Koch+Koch+Koch+Koch+Koch	75	75	75
Abrahamson+Katz+Koch+Koch+Koch+Koch+Koch+Koch+Koch+Koch+Koch+Koch+Koch+Koch+Koch	80	80	80
Abrahamson+Katz+Koch+Koch+Koch+Koch+Koch+Koch+Koch+Koch+Koch+Koch+Koch+Koch+Koch+Koch	85	85	85
Abrahamson+Katz+Koch+Koch+Koch+Koch+Koch+Koch+Koch+Koch+Koch+Koch+Koch+Koch+Koch+Koch+Koch	90	90	90
Abrahamson+Katz+Koch+Koch+Koch+Koch+Koch+Koch+Koch+Koch+Koch+Koch+Koch+Koch+Koch+Koch+Koch+Koch	95	95	95
Abrahamson+Katz+Koch+Koch+Koch+Koch+Koch+Koch+Koch+Koch+Koch+Koch+Koch+Koch+Koch+Koch+Koch+Koch+Koch	100	100	100

Ginkgo

The Ginkgo parallel linear algebra package now has the solvers and preconditioners we need, with support for multi-GPU nodes. This graph shows how a Ginkgo BICGStab solver scales on the Frontier supercomputer (AMD MI250X accelerators).

$$\begin{cases}
 \nabla \cdot (\sigma \nabla \phi) = I_s & \text{on } \Omega^i \\
 \nabla \cdot (C \nabla \phi) = 0 & \text{on } \Omega^e \\
 V_m = \phi^i - \phi^e & \text{on } \Gamma_m \\
 -C \nabla \phi^i \cdot \mathbf{n} = C_m \nabla V_m \cdot \mathbf{n} = C_m \nabla V_m \cdot \mathbf{n} + J_{ion}(V_m, \mathbf{y}) = J_s & \text{on } \Gamma_m^i \text{ (transmem. currents)} \\
 -C \nabla \phi^e \cdot \mathbf{n} = C \nabla \phi^i \cdot \mathbf{n} - J_{ion}(V_m, \mathbf{y}) + \sigma (\phi^i - \phi^e) & \text{on } \Gamma_m^e \text{ (intercalated discs)} \\
 C_m \nabla V_m \cdot \mathbf{n} = J_s & \text{on } \Gamma_e \text{ (electrode surface)} \\
 \phi(\mathbf{y}) = \phi(V_m, \mathbf{y}) &
 \end{cases}$$


Mmg PLATFORM

We improved the Mmg remeshing software so that it can handle our complex multi-domain meshes. This allowed us to make virtual cardiac tissue samples upto 1 mm³ volume (7843 cells, 352 million tetrahedra, 115 thousand internal boundaries). We are working to achieve this also with the parallel version of Mmg, and then to scale up further.

StarPU

The StarPU runtime scheduler is used to balance load between CPU and GPU.

openCARP

The code is based on the widely used openCARP software for cardiac simulation. We enhanced openCARP with a Ginkgo back-end, asynchronous parallel output, and many other upgrades.

MEGWARE

HPC manufacturer MEGWARE provides a development platform that allows fine-grained measurement of energy consumption.