Simulations of Complex Systems using WebGL and HTML5: Exploiting Your Computer's GPUs for Real Time and Platform-Independent Interactive Calculations

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Motivation (abstraction)

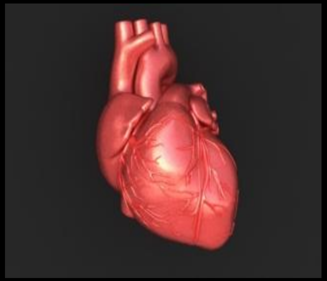
Computational Model
Linear Hybrid Automata (LHA), Kripke structure, etc.

Formal Analysis – Exhaustive exploration of state space

Model Checking (MC), Abstract Interpretation (AI), Parameter Estimation.

Qualitative/ Quantitative Insights (Abstract parameter and state-space)

Hybridization, over-approximation, abstraction



Biological Phenomena
(Cardiac excitation: cell & tissue-level behavior)

Mathematical Modeling

$$\frac{\partial x_i}{\partial t} = f_i(t, x_1(t), x_2(t) \ldots x_n(t)) + \nabla$$

Mathematical Model
(Possibly Non-linear)

Minimal Model (ABSTRACT)
Variables: 4
Parameters: 27

Tusscher-Noble-Panfilov-03
Variables: 17
Parameters: 44

Intermediate Models

Systematic Refinement

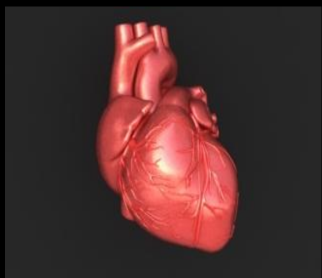
Abstraction

Iyer Model (DETAILED)
Variables: 67
Parameters: 94

Tower of Abstraction for Cardiac Models

Physiological Insights
- Root-cause detection
- Personalized treatment
- Pharmacology

Motivation
(Model Checking)



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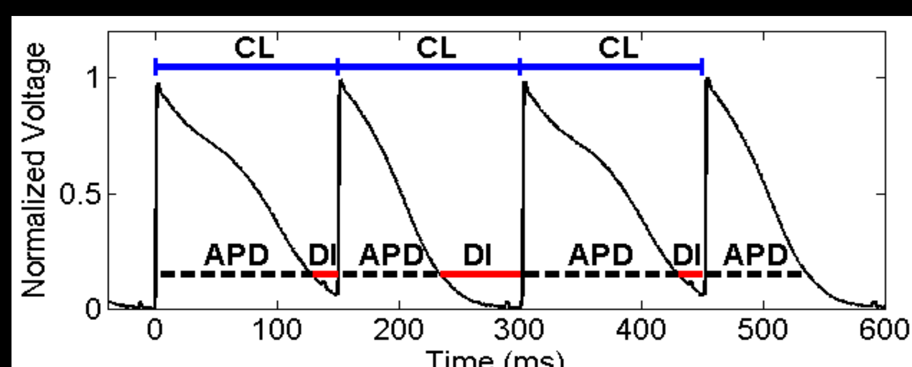
Mathematical Modeling →

$$\frac{\partial x_i}{\partial t} = f_i(t, x_1(t), x_2(t) \ldots x_n(t)) + \nabla$$

Mathematical Model

Model Checking
Mathematical cell models -------------------------→ normal or disease

- Model of cardiac cell and excitability (useful for example ischemia characterization) ✔
- Alternans in time and space (temporal and spatial extension of Model checking)



Motivation

During Model Checking and Abstract interpretation of cardiac models
We still need to solve complex and reduced models for comparison

CMACS: We aim to gain fundamental new insights into the emergent behavior of complex biological and embedded systems through the use of revolutionary, highly scalable and fully automated modeling and analysis techniques

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Modeling with GPU

Motivation

Modeling with GPU

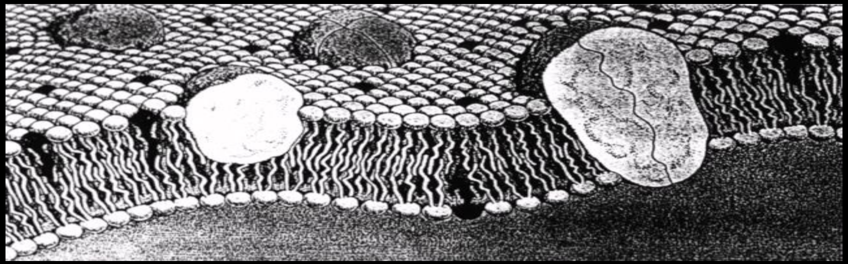
A Graphics Processing Unit (GPU) is a specialized electronic circuit designed to rapidly access and manipulate memory to accelerate the generation of images for fast output to a display.

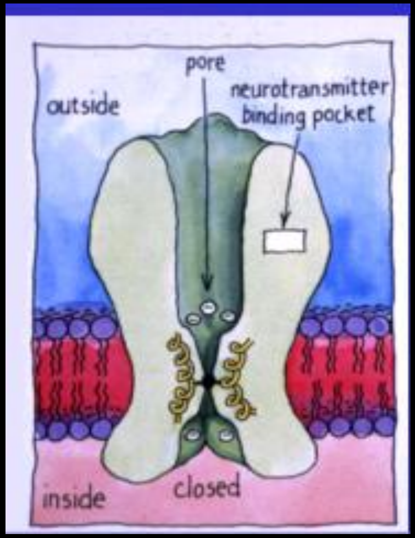
Over the past decade due to its massively parallel architecture structure it has become a mean to accelerate general purpose scientific and engineering computing.

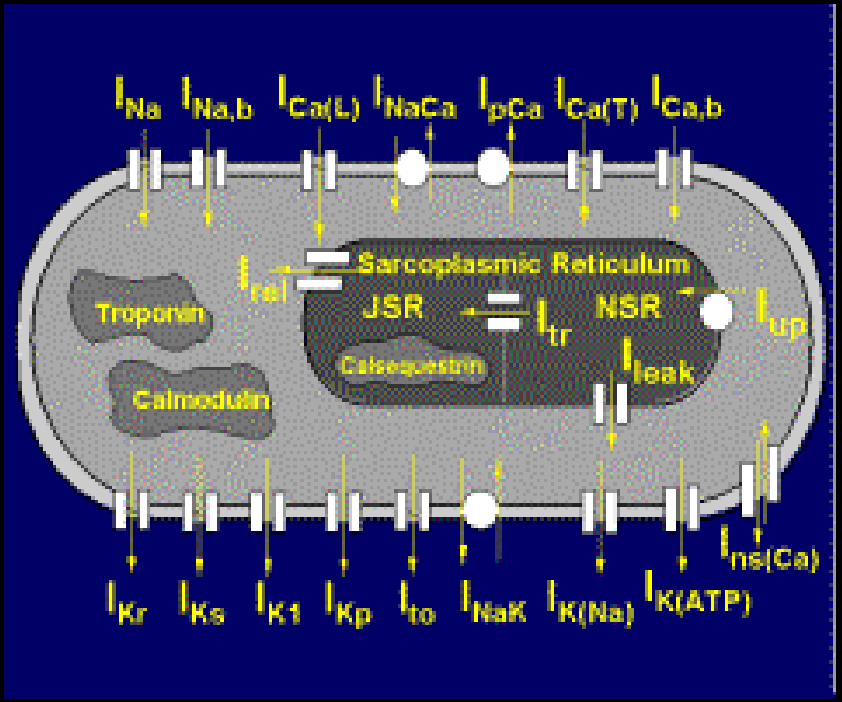
WebGL is a new web-based cross-platform technology that allows the execution of JavaScript and Shader codes directly to a computer's GPU from a web browser without the need for any plug-ins.

Therefore it is now possible to run high-performance parallel computing simulations over the web on a local PC or laptop independent of the operating system used.

Membrane Potential Models







Membrane Potential Models

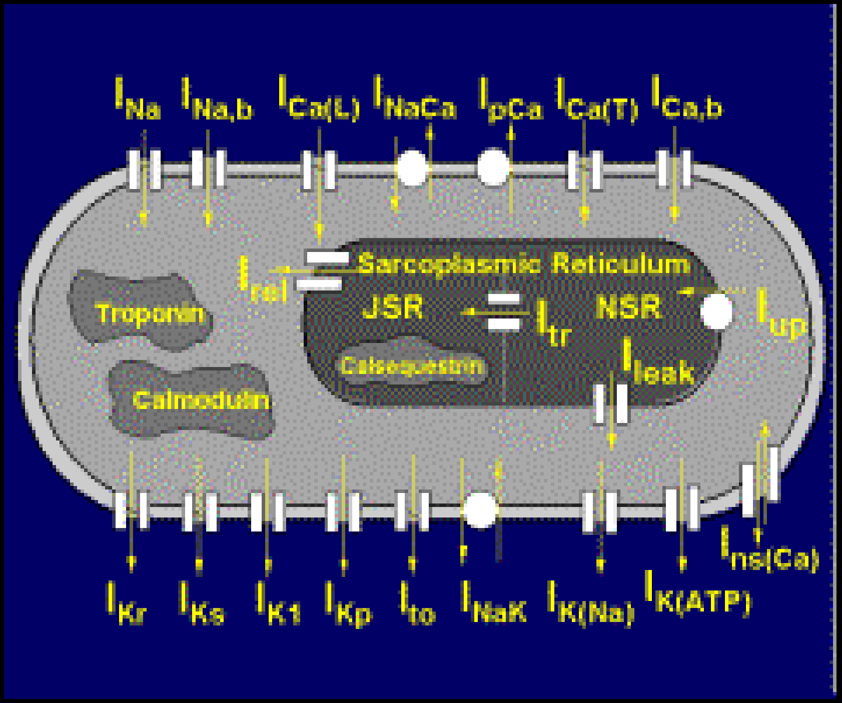
About 92 models developed so far for mammalian cardiac cells

- Noble model. 1962; 4 ODEs
  (Generic Purkinje myocyte)

- Beeler-Reuter model. 1977; 8 ODEs
  (Generic ventricle myocyte)

- Hund-Rudy model. 2004; 29 ODEs
  (Canine, ventricle, myocyte)

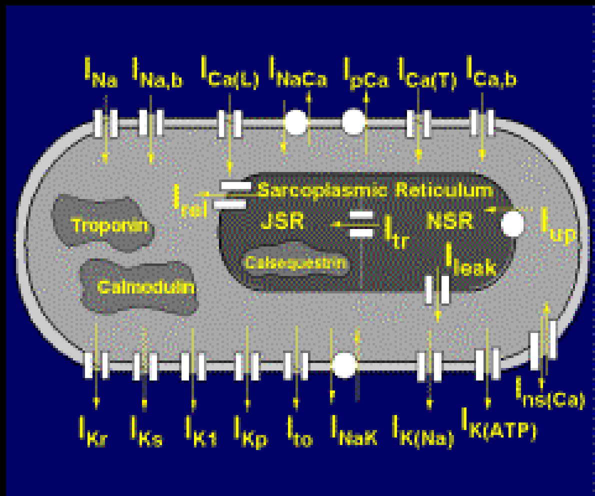
- Iyer et al. model. 2007; 67 ODEs
  (Human, ventricle, myocyte)

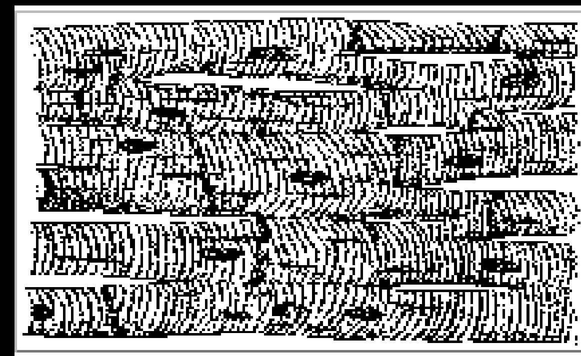


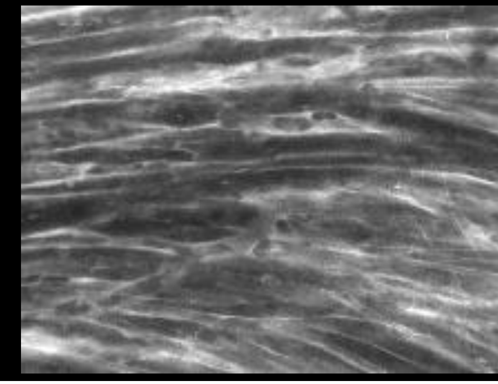
- Fenton-Karma model. 1998 (2008); 3 (4) ODEs
  (minimal model that fits to experiments and other models)

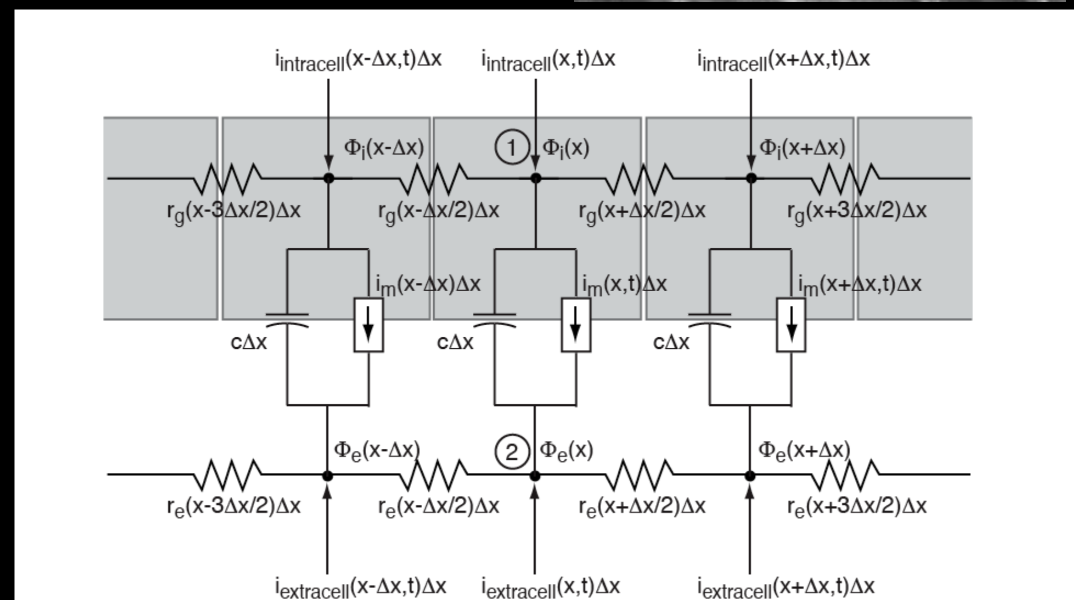
Fenton and Karma (1998), Chaos 8;20-47
Bueno, Cherry and Fenton (2008), JTB 253; 544-560
Flavio H Fenton and Elizabeth M. Cherry (2008), Scholarpedia, 3(8):1868

Electrical Waves in Tissue









Cardiac tissue is a reaction-diffusion system.

$$V_m = \phi_i - \phi_e,$$

$$\nabla(\sigma_i \nabla \phi_i) = I_m = \beta_{sv}\left(C_m \frac{\partial}{\partial t} V_m + I_{ion}\right),$$

$$\nabla(\sigma_e \nabla \phi_e) = I_m = \beta_{sv}\left(C_m \frac{\partial}{\partial t} V_m + I_{ion}\right),$$

$$\nabla \sigma_b \nabla \phi_b = -I_{stim}.$$

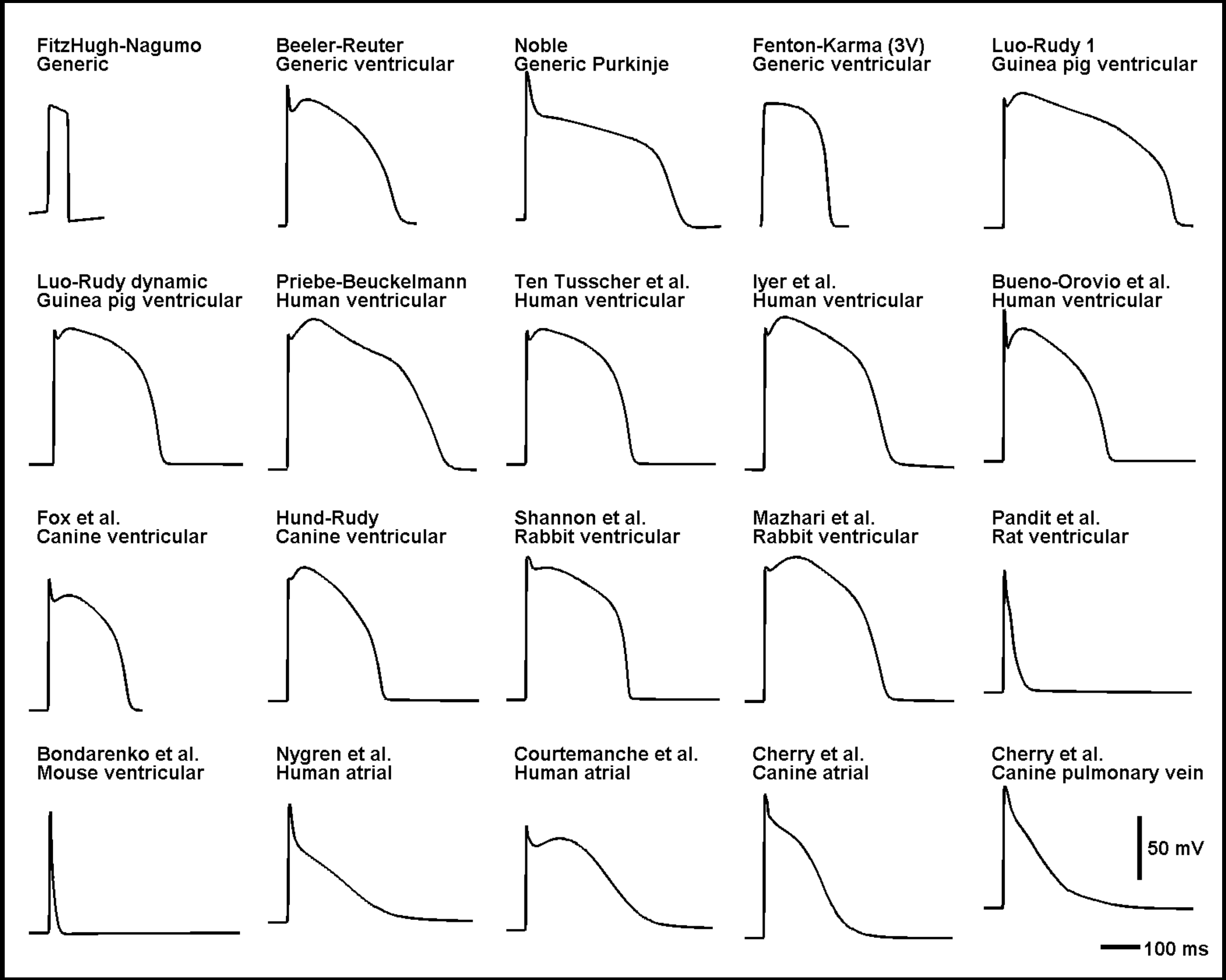
$$n(\sigma_i \nabla \phi_i) = 0,$$

$$n(\sigma_e \nabla \phi_e) = n(\sigma_b \hat{I}) \nabla \phi_i,$$

$$\phi_e = \phi_b,$$

Many models for diverse cell types

Implemented (~40) most of the existing ionic models in single cell and in tissue



Models of cardiac cell
Flavio H Fenton and Elizabeth M. Cherry (2008), Scholarpedia, 3(8):1868.

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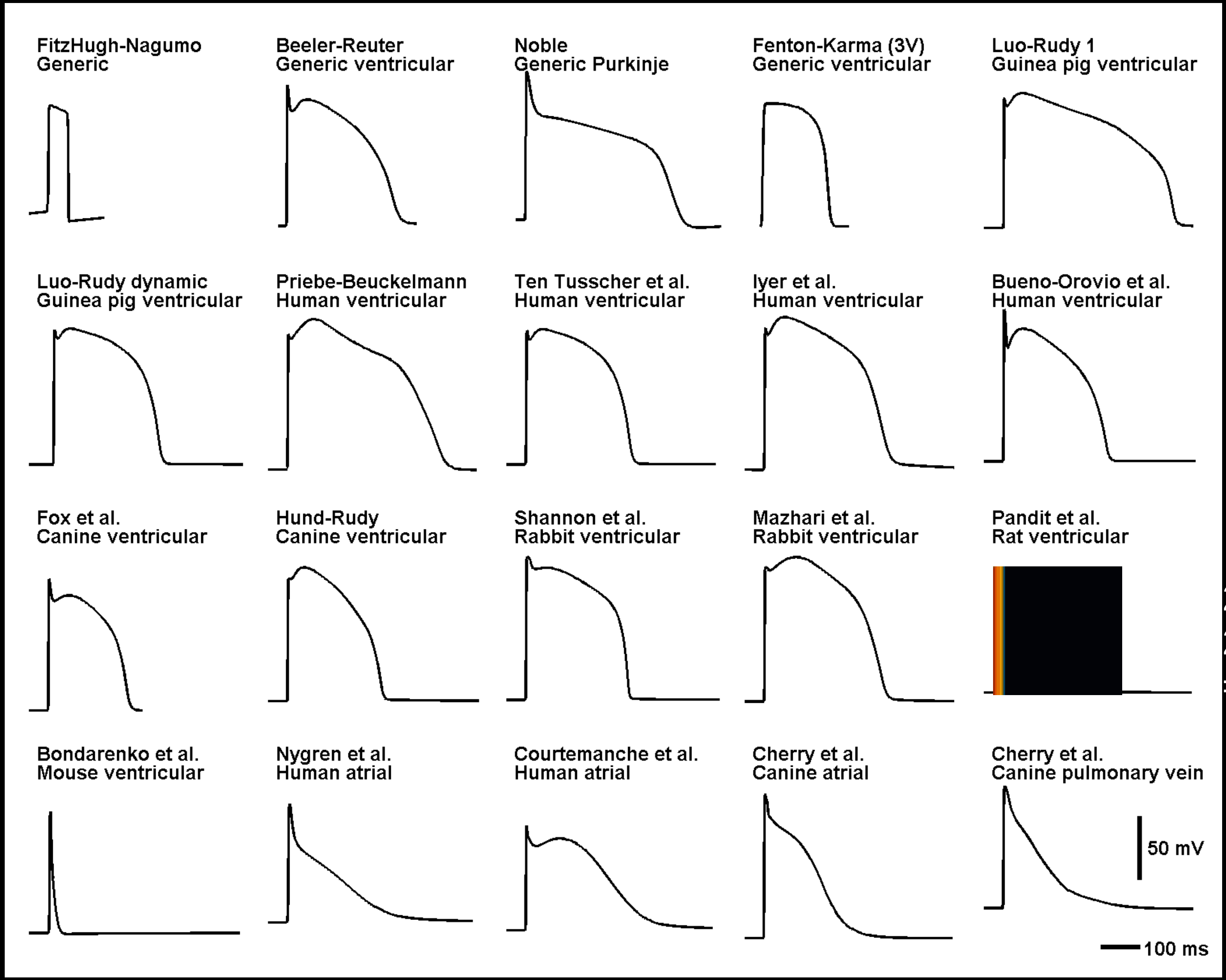

26 variables
2D (200x200x26
=1040000)

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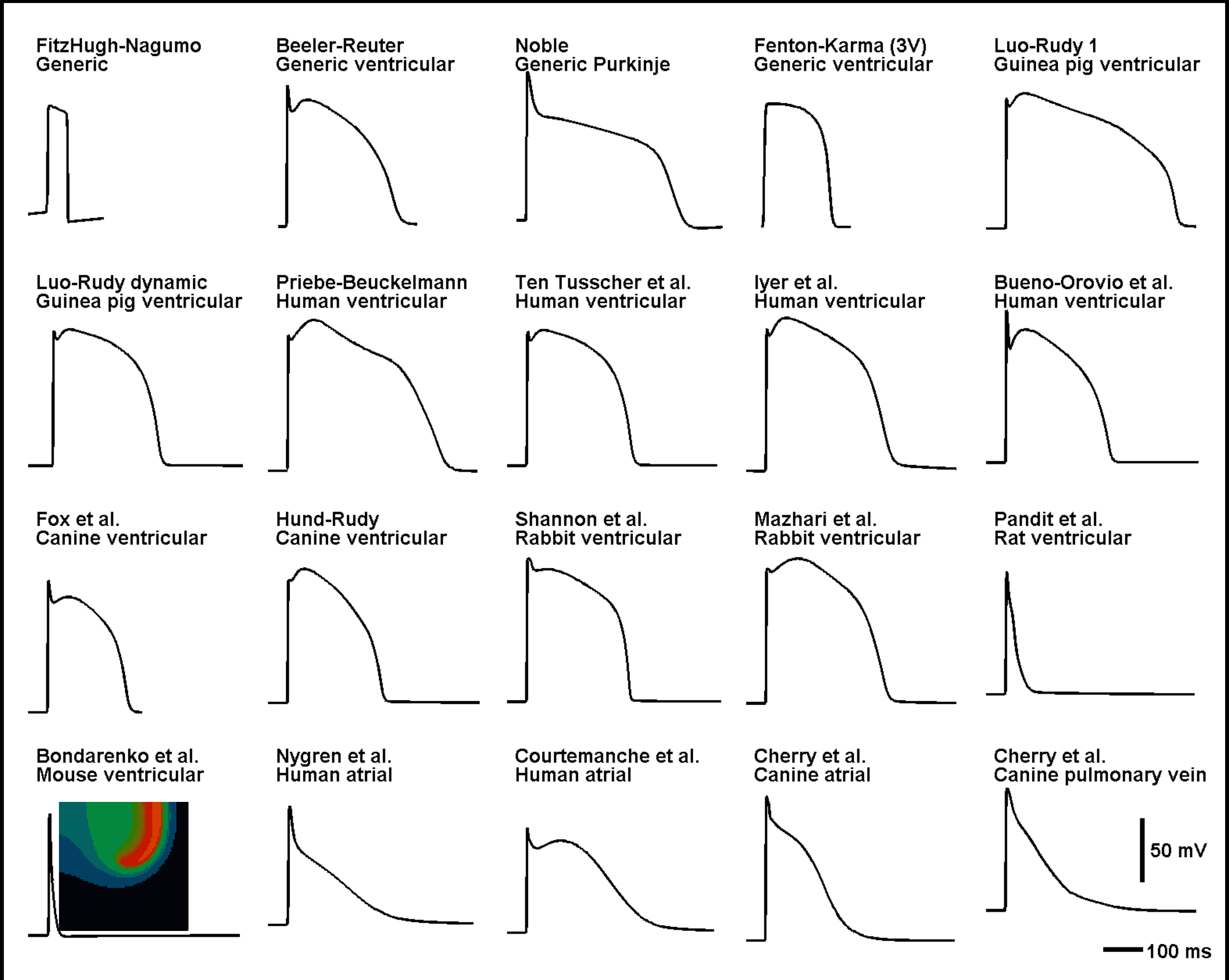

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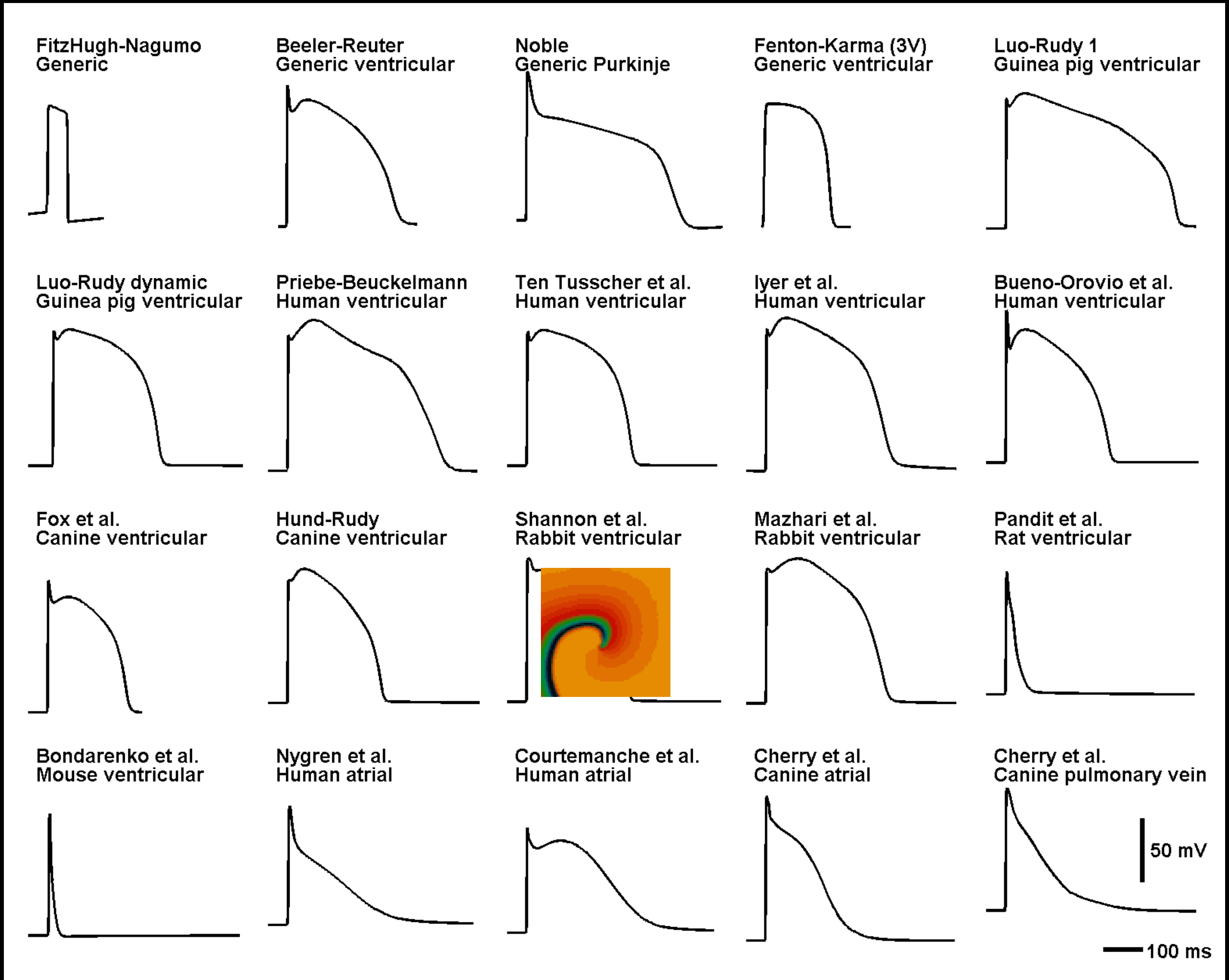

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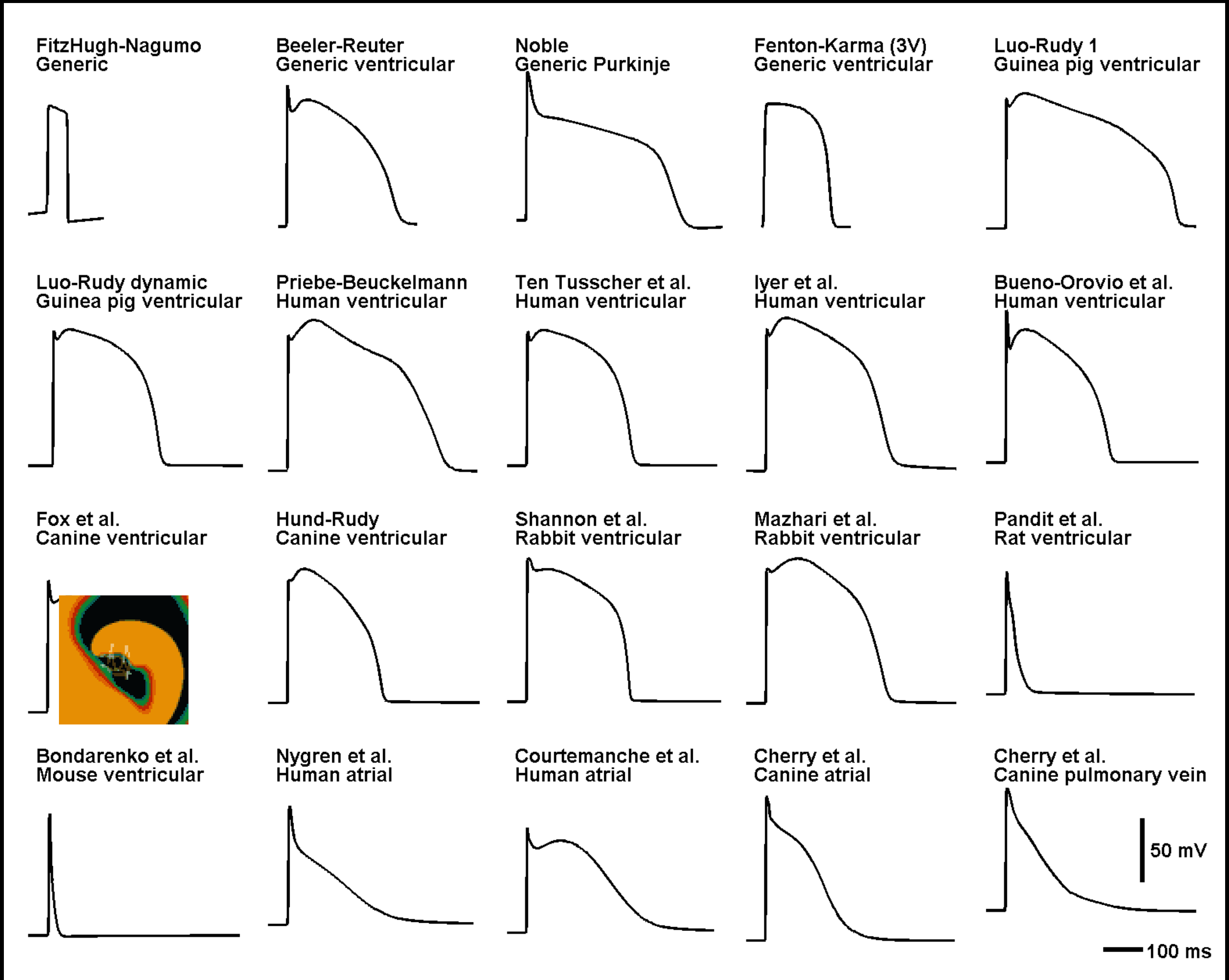

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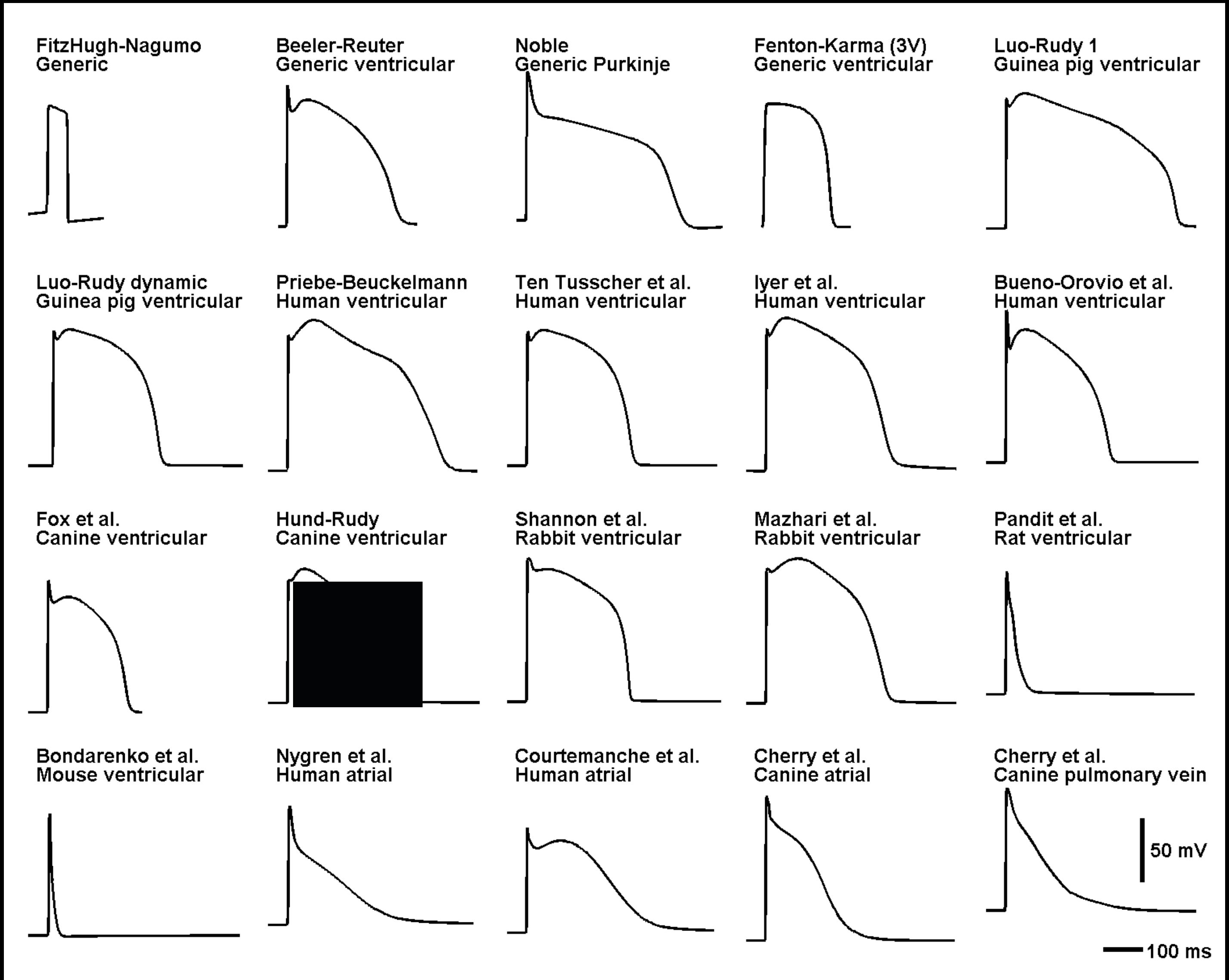

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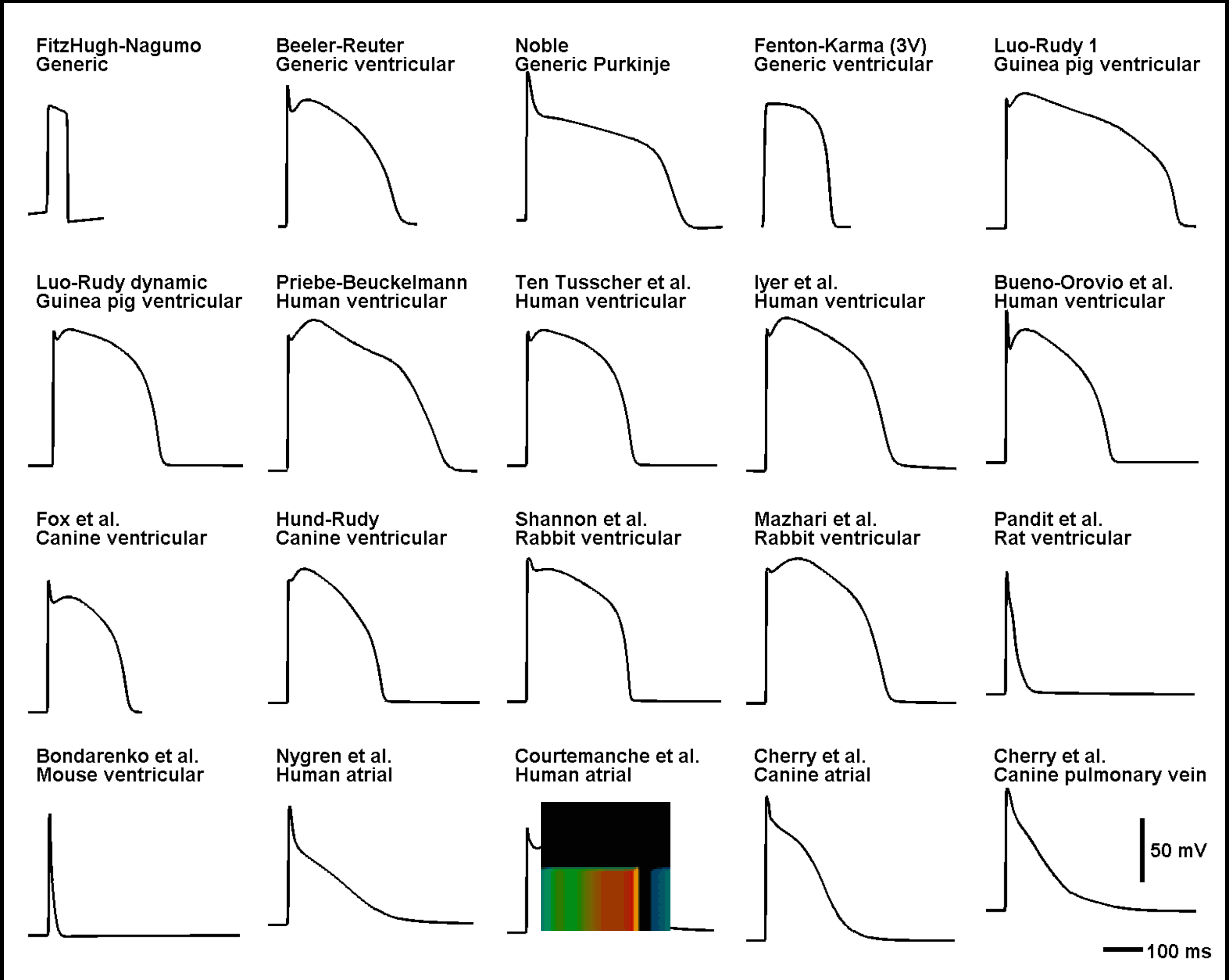

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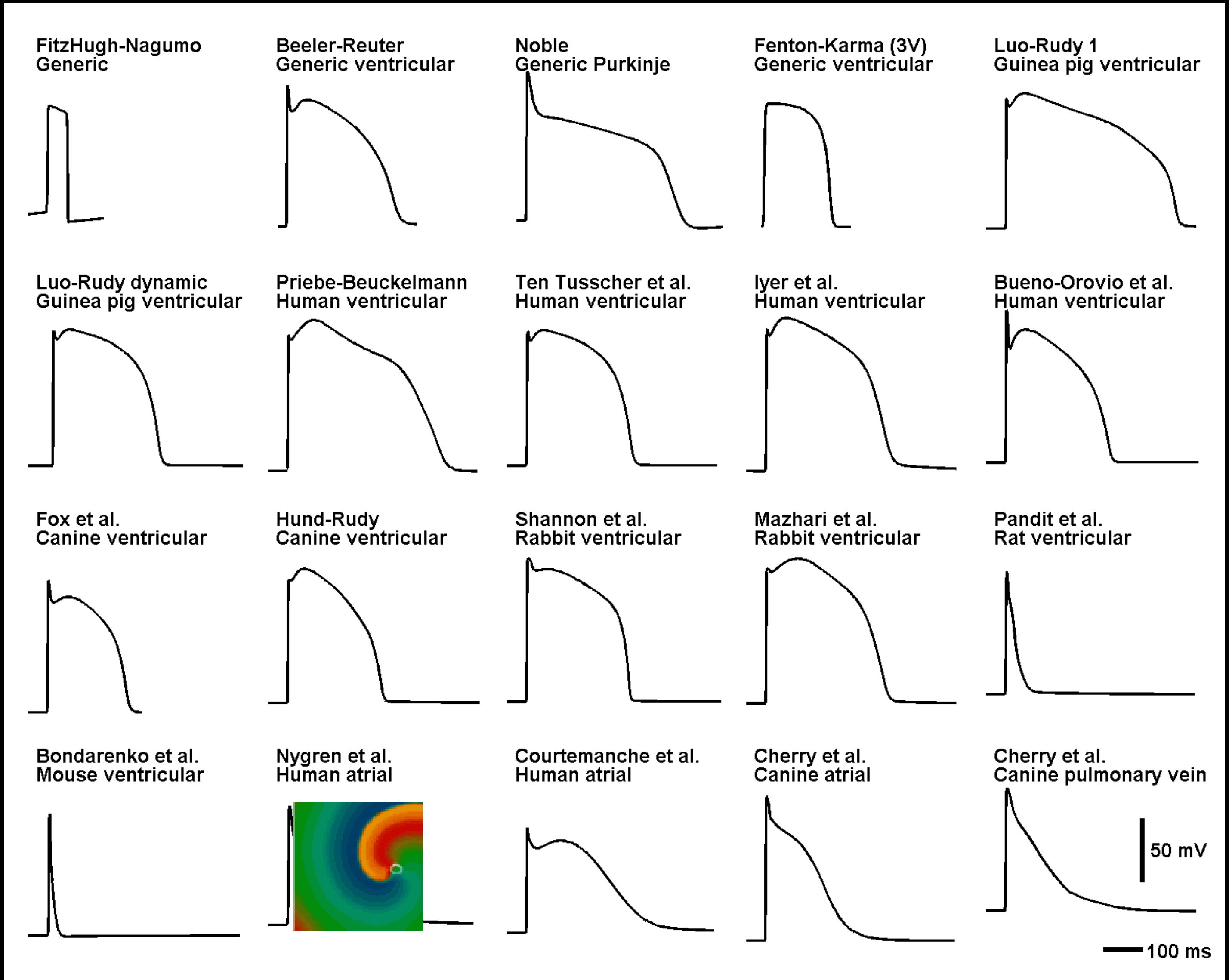

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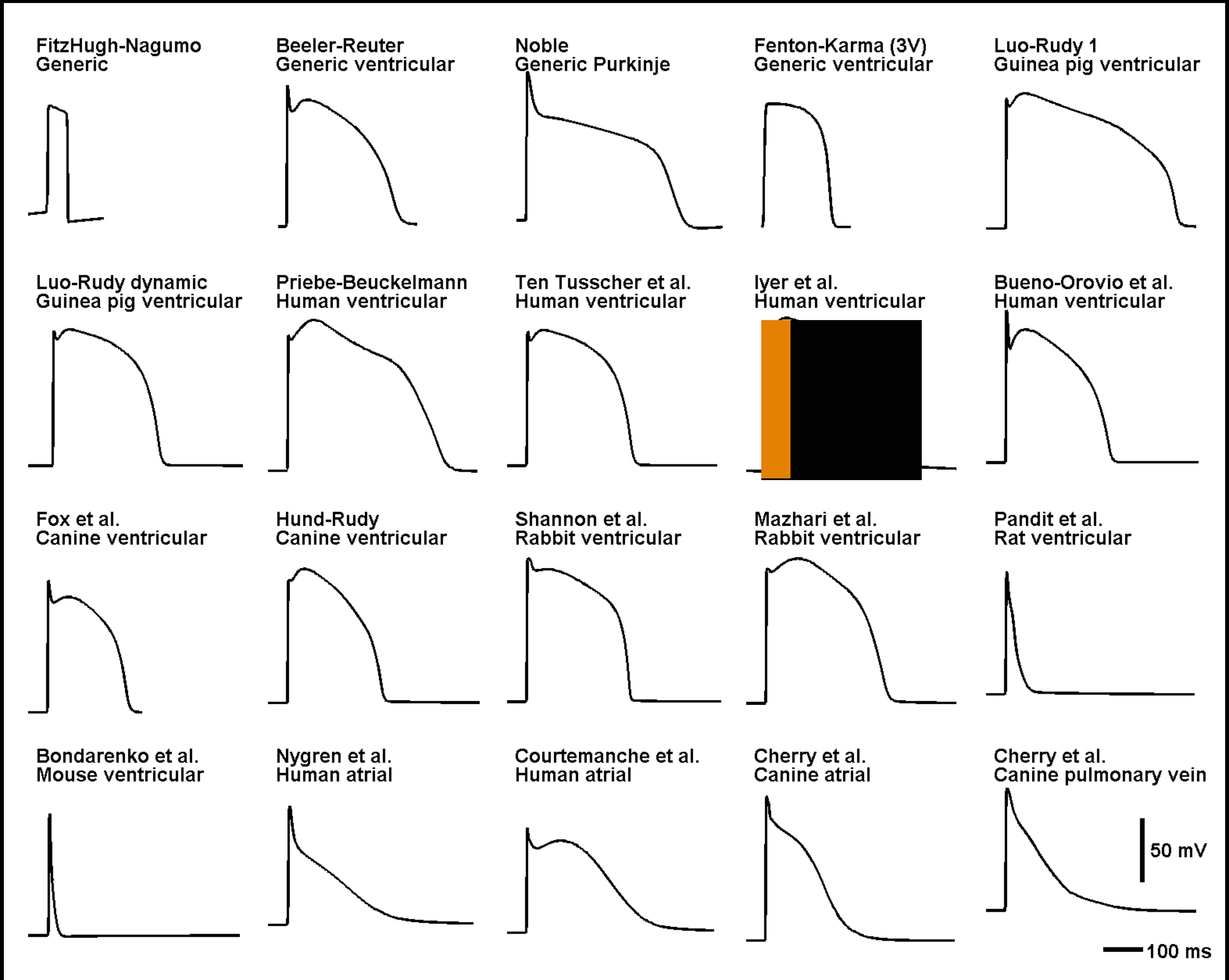
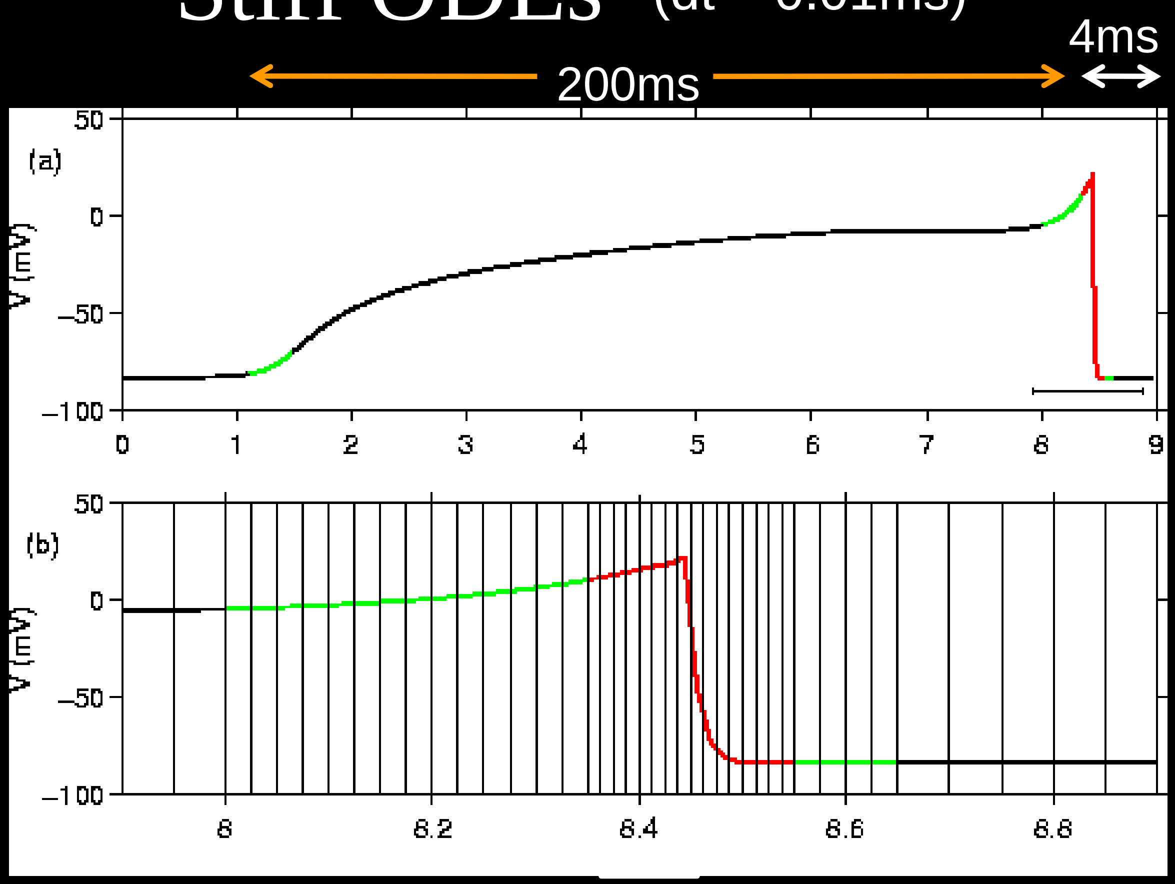


67 variables
2D (200x200x67
=2680000)

Models of cardiac cell
Flavio H Fenton and Elizabeth M. Cherry (2008), Scholarpedia, 3(8):1868.

Modeling and simulations challenges

- Stiff ODEs (dt ~ 0.01ms)

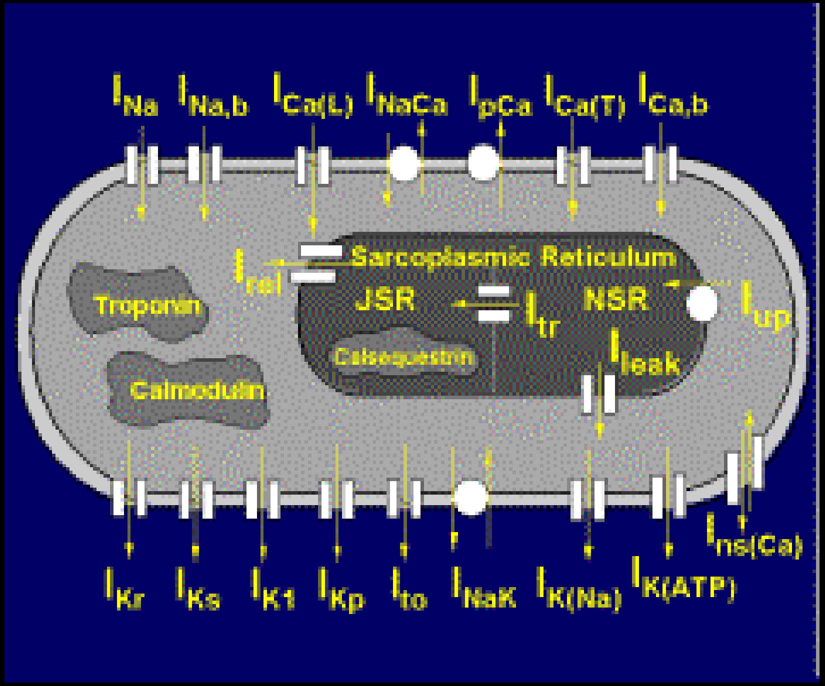


Adaptive mesh refinement or semi implicit methods

Modeling and simulations challenges

- Stiff ODEs (dt ~ 0.01ms)

- Number of ODEs per cell
  ~(4 – 100)

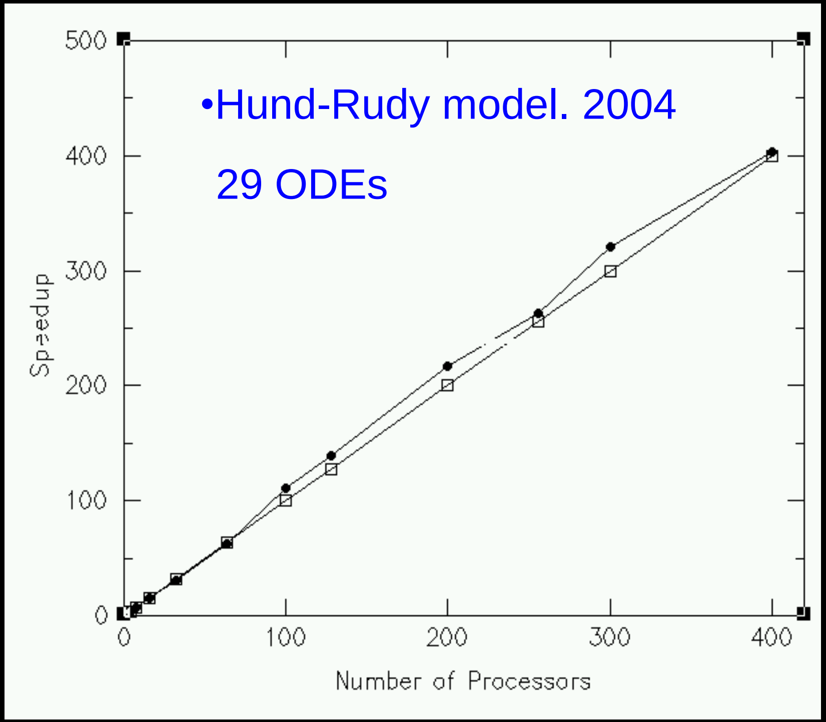


[4 --100]
depending on the model

Cherry and Fenton, Pitt. Sup. Ctr. 2010. Proj. Sci. Comp. pg 28-31. January 2011.

Modeling and simulations challenges

- Stiff ODEs (dt ~ 0.01ms)
- Number of ODEs per cell
  ~(4 – 100)
- Number of cells simulated



~200 microns minimum spatial resolution

GPU instead of CPU

simulation on a 4cmx4cm (200x200) x 4 = 160,000 ODE equations
100 = 4,000,000 ODE equations

Hund-Rudy model (29 ODEs) 1 second of simulation in 2d
1,160,000 x100,000 = 1.16 $\times 10^{11}$ ODE equations

1 second of simulation in 3d : ~ twenty trillion ODE equations

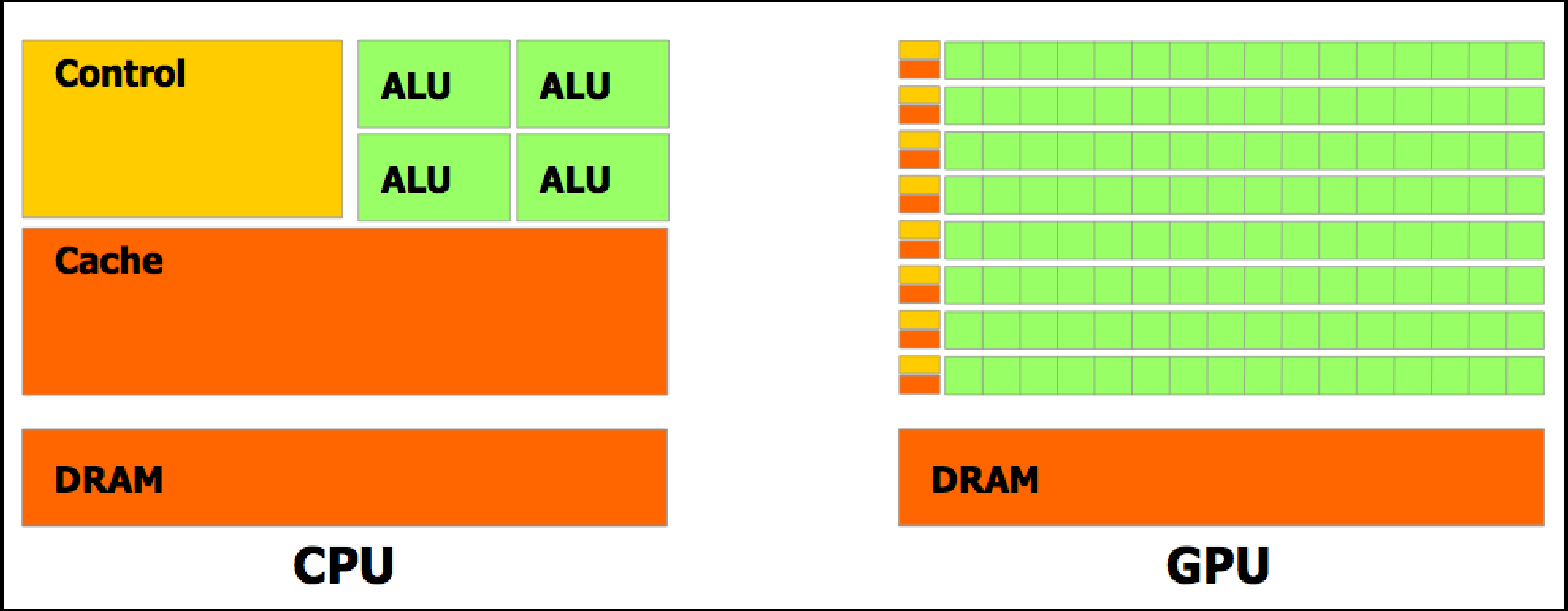
Cherry and Fenton, Pitt. Sup. Ctr. 2010. Proj. Sci. Comp. pg 28-31. January 2011.

GPU simulations

GPUs (Graphics Processing Units) have evolved far beyond single processors. Modern NVIDIA GPUs are not single processors but rather are parallel supercomputers on a chip that consist of very many, very fast processors. Contemporary NVIDIA GPUs range from 16 to 480 stream processors per card,

Available Technologies

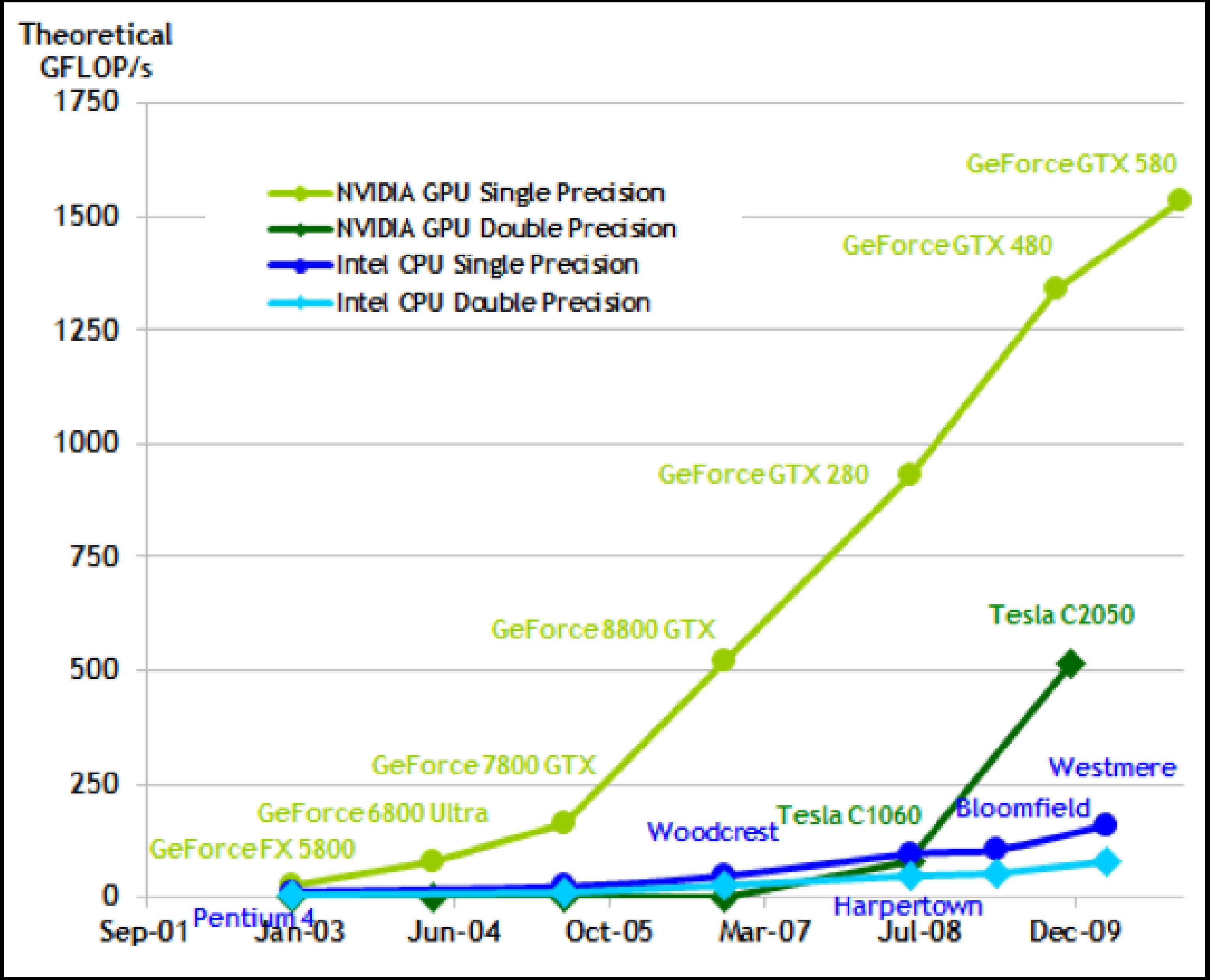
CPU based | GPU based



The GPU devotes more transistors to data processing

This image is from CUDA programming guide

GPU vs CPU


Theoretical GFLOP/s
1750
1500
1250
1000
750
500
250
0
NVIDIA GPU Single Precision
NVIDIA GPU Double Precision
Intel CPU Single Precision
Intel CPU Double Precision
GeForce GTX 580
GeForce GTX 480
GeForce GTX 280
GeForce 8800 GTX
Tesla C2050
GeForce 7800 GTX
GeForce 6800 Ultra
GeForce FX 5800
Westmere
Bloomfield
Tesla C1060
Woodcrest
Harpertown
Pentium 4
Sep-01
Jan-03
Jun-04
Oct-05
Mar-07
Jul-08
Dec-09

Tesla C1060

30 Multiprocessors
240 Cores
Processor core clock: 1.296 GHz
933 Gigaflops (Single precision)
78 Gigaflops (Double Precision)
Max Bandwidth(102 Gigabytes/sec)
4 GB of DRAM

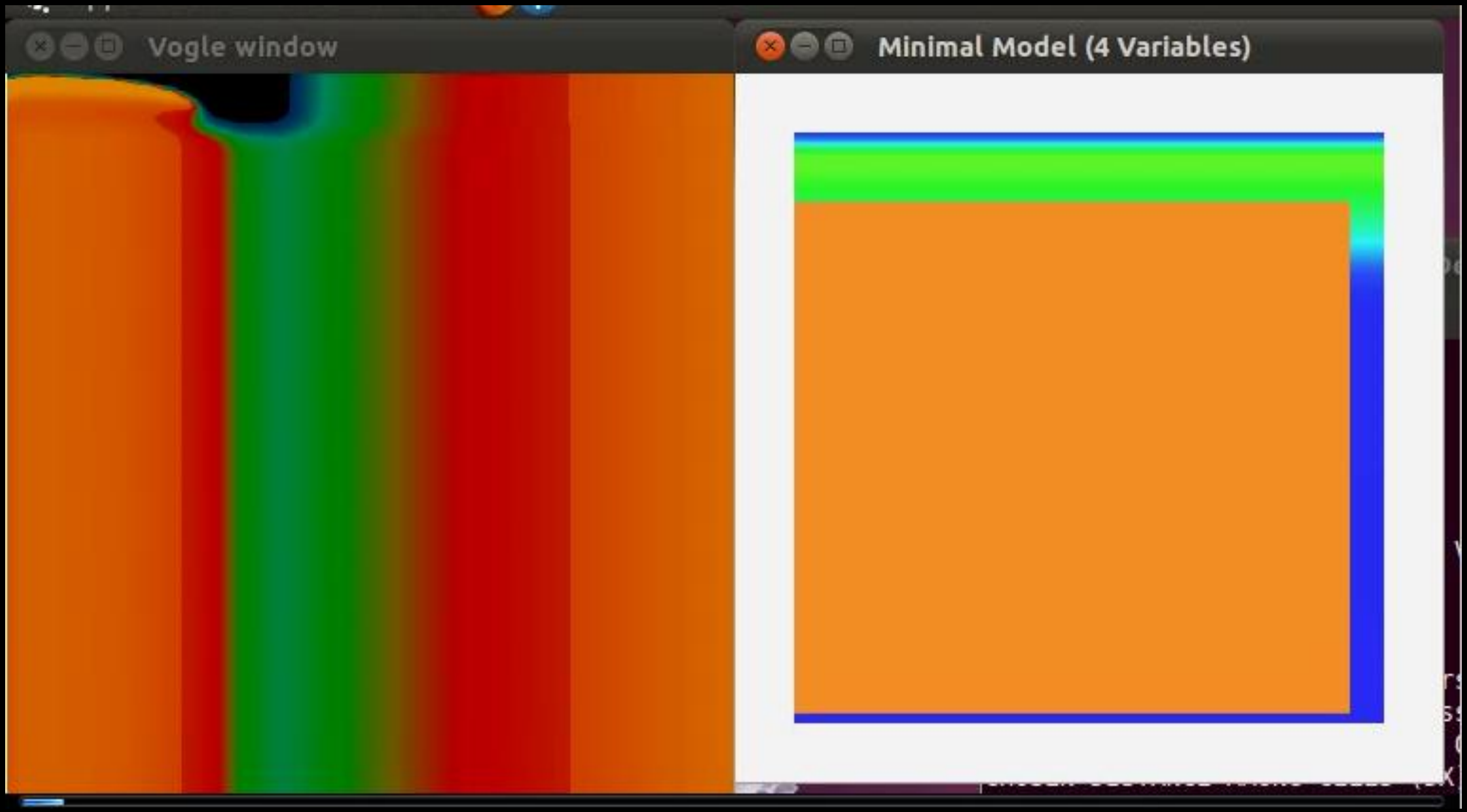
Cost: **1000 $**

Fermi C2070

14 Multiprocessors
448 Cores
Processor core clock: 1.15 GHz
1030 Gigaflops (Single precision)
515 Gigaflops (Double precision)
Max Bandwidth (144 GBytes/sec)
6 GB of DRAM

Cost: **3200 $**

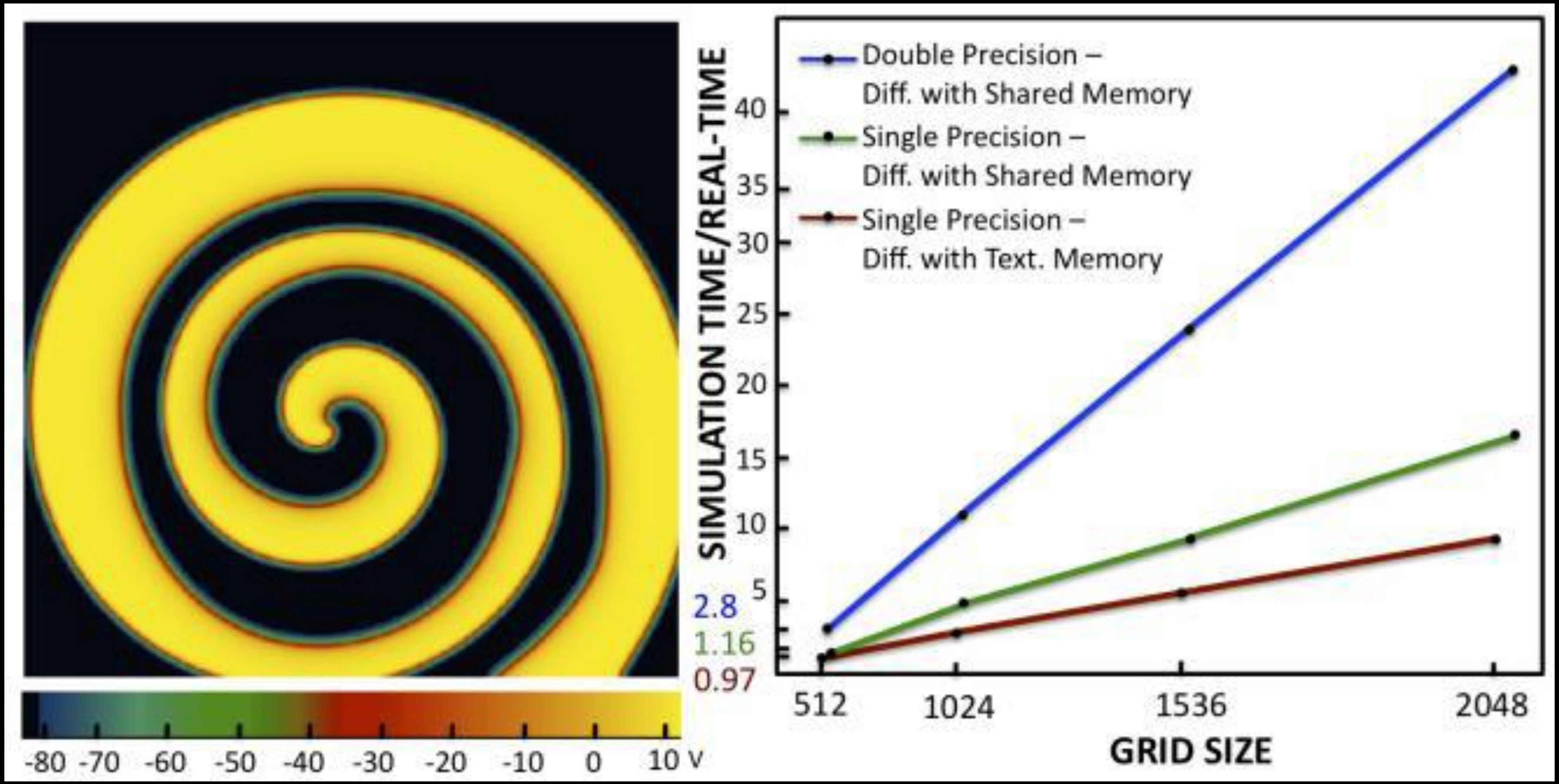
GPU near-realtime simulations



CPU (12.8x12.8 cm^2) GPU

Same machine

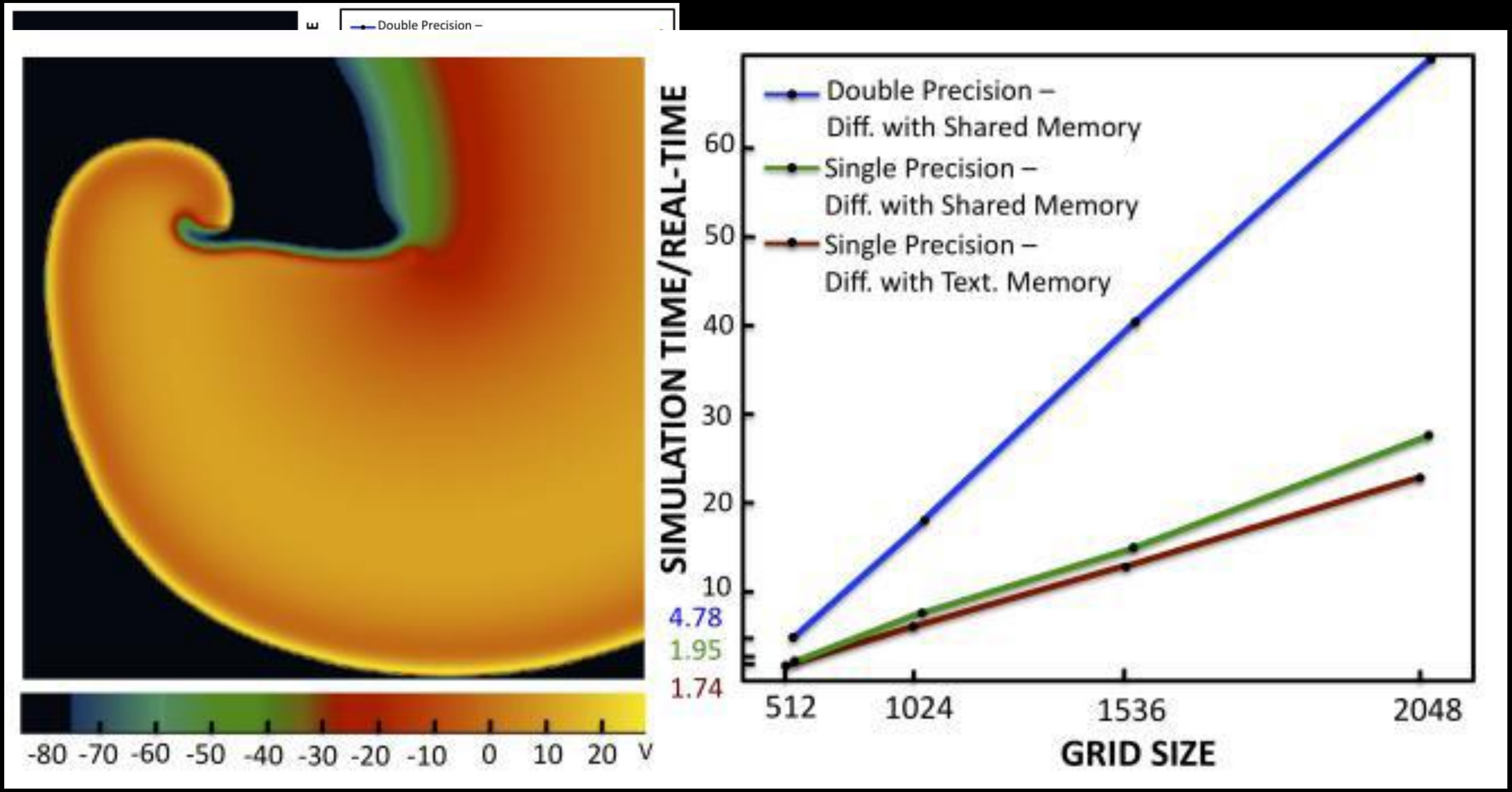
GPU near-realtime simulations



2^18 (12.8x12.8 cm2) → 2^22 : ~4.2million nodes

2V Karma model

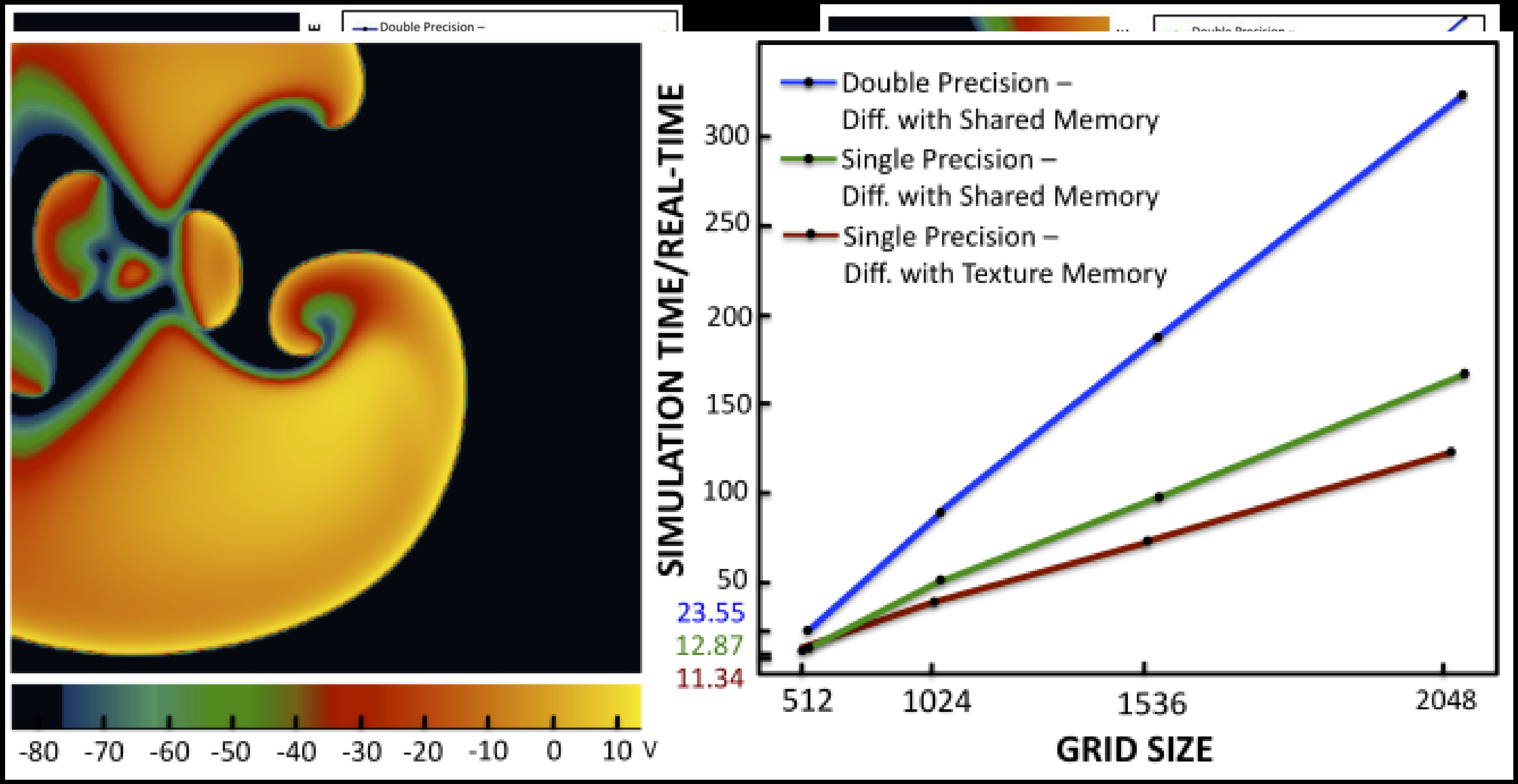
GPU near-realtime simulations



2^18 (12.8x12.8 cm2) → 2^22 : ~4.2million nodes

4V Minimal model

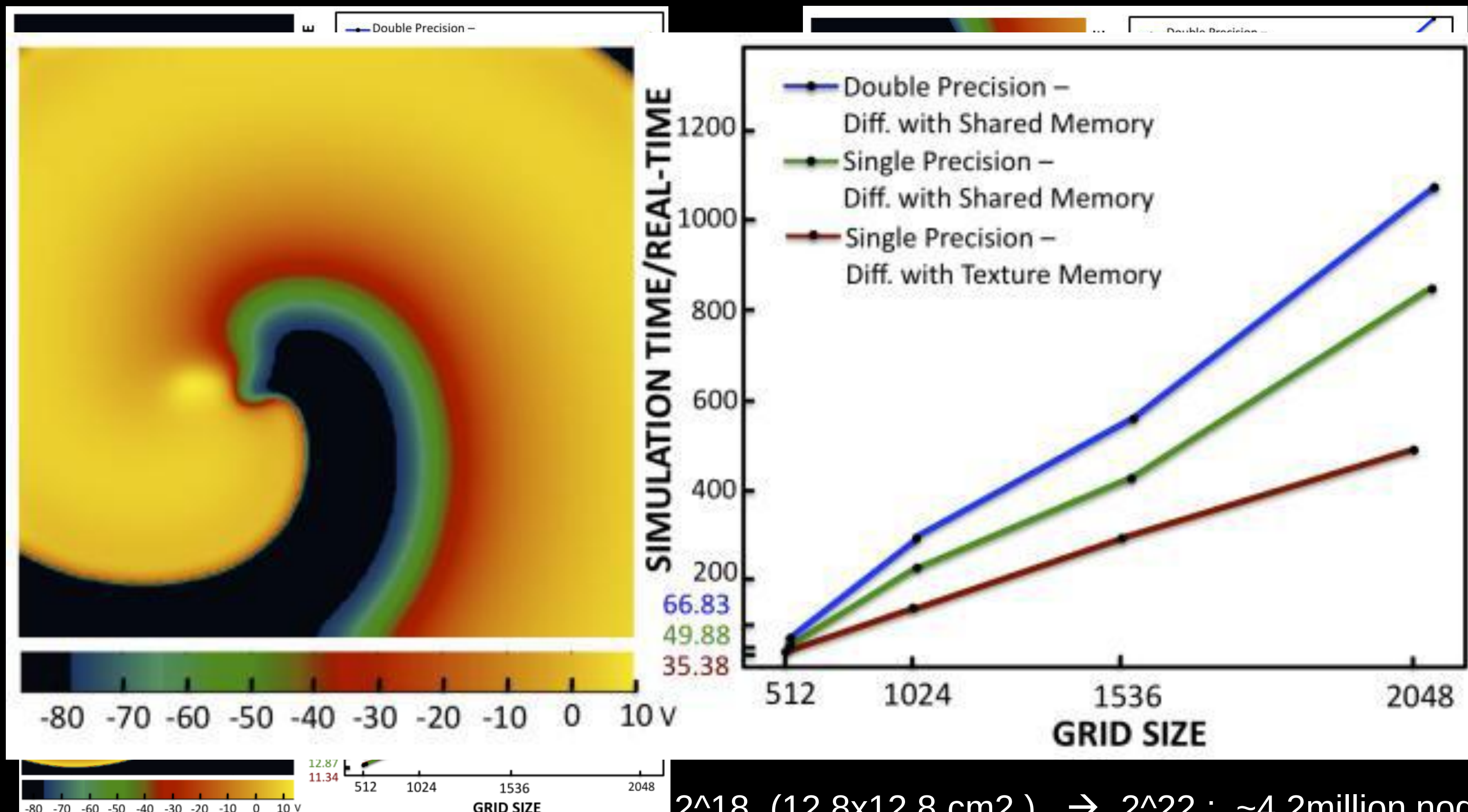
GPU near-realtime simulations



2^18 (12.8x12.8 cm2) → 2^22 : ~4.2million nodes

8V BR model

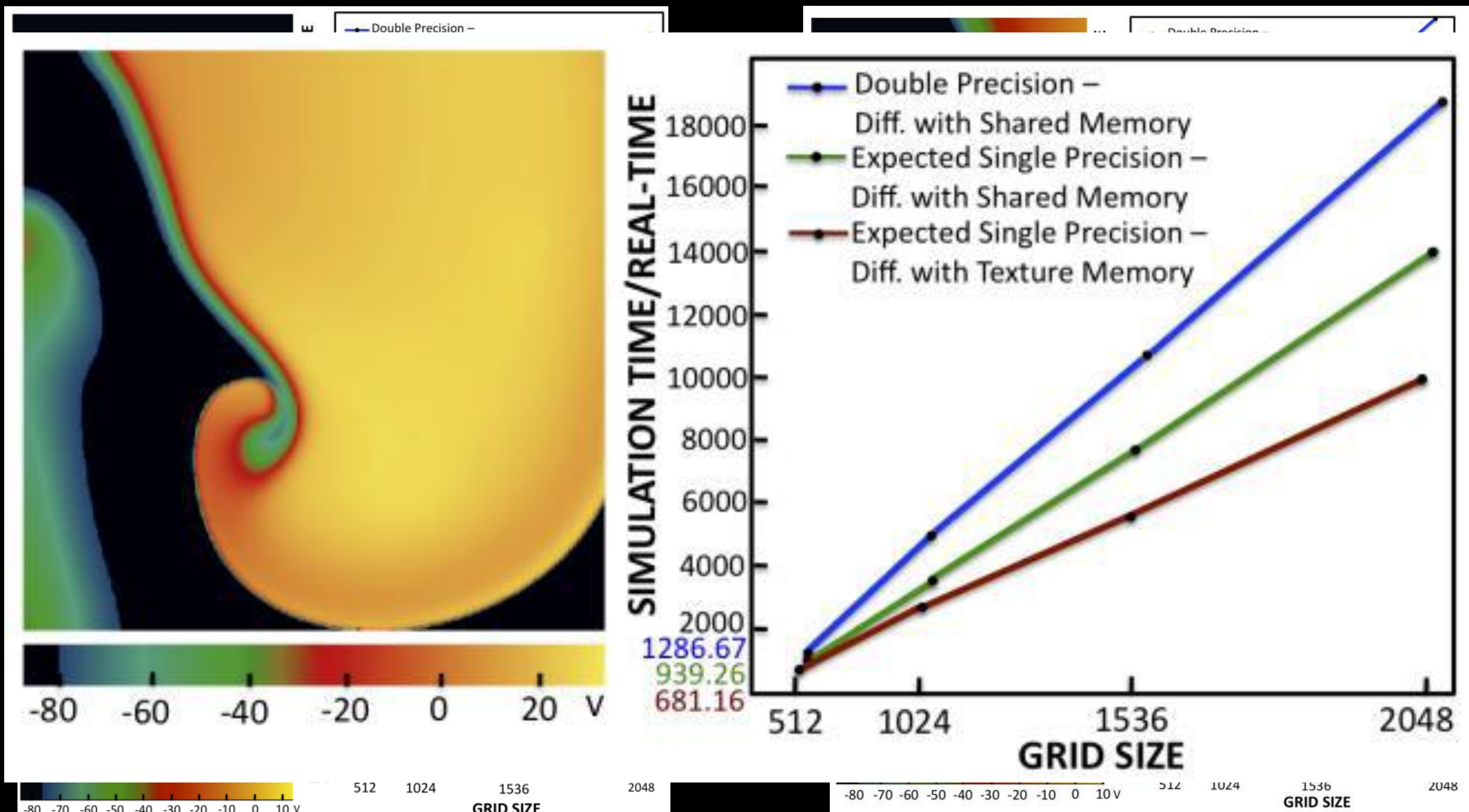
GPU near-realtime simulations



2^18 (12.8x12.8 cm2) → 2^22 : ~4.2million nodes

19V TP model

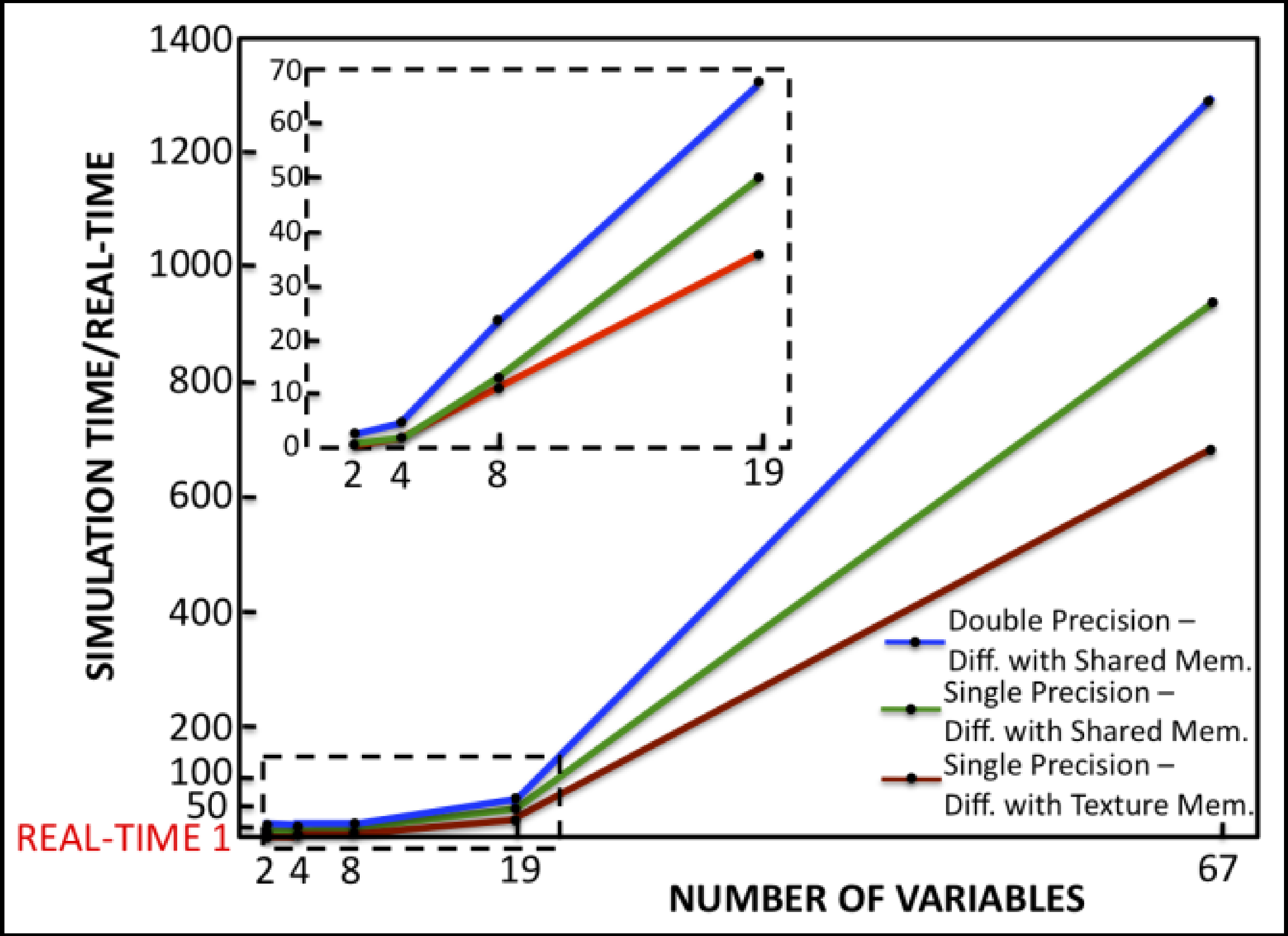
GPU near-realtime simulations



67V Iyer et al, model

2^18 (12.8x12.8 cm2) → 2^22 : ~4.2million nodes

GPU near-realtime simulations



WebGL + HTML5

- **WebGL** (*Web Graphics Library*) uses JavaScript, Shader language and OpenGL for interactive simulations within any compatible web browser without the use of plug-ins.

Browsers supporting WebGL: Google Chrome
Fire Fox, Mozilla (permission)

Examples of reaction diffusion models with WebGL in 2D

- Multiple spiral waves (chaos). 2V Barkley model
- Spiral wave (2V Karma model) interaction with the code
- 1962 Noble Model (tip trajectory and breakup)

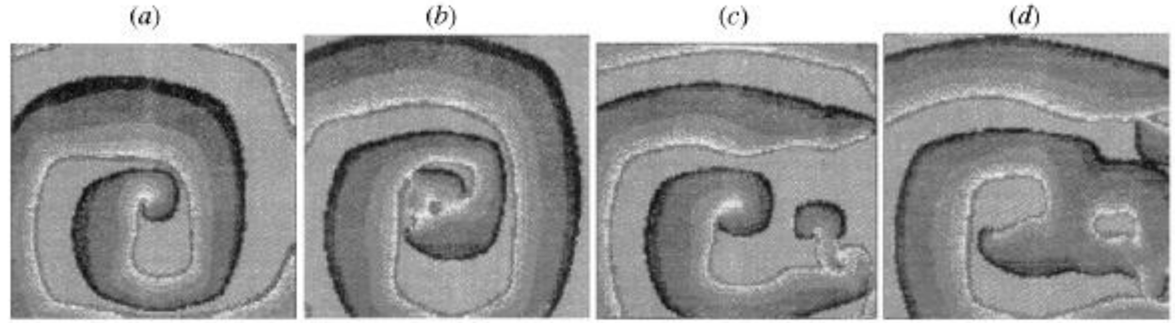


Figure 1. Spiral breakup in a Noble (1962) model of cardiac tissue. Reproduced from Panfilov & Holden (1990) with permission from Elsevier Science. Sequential snapshots of potential distribution: (a) $t = 1720$ ms; (b) $t = 1880$ ms; (c) $t = 2920$ ms; (d) $t = 3080$ ms. Potentials are coded in equal 10 mV steps, from -85 mV (dark) to $+5$ mV (white).

Examples of reaction diffusion models with WebGL in 2D

- Minimal model of Human AP
- Beeler Reuter model (1977) Super computer Winfree 1991
- 3D simulations, (scroll waves, breakup in 3d)
- GPU for other CMACS problems?