Parallelization of Jacobi Algorithm for Solving Laplace equation

...and my attempt at parallelization of my cell project

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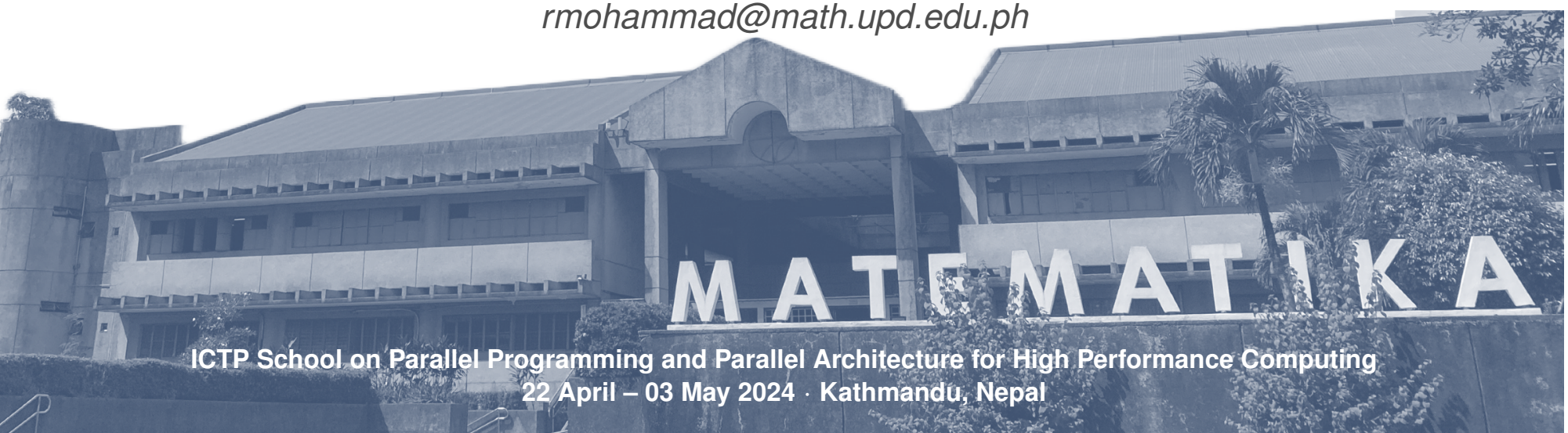

ICTP School on Parallel Programming and Parallel Architecture for High Performance Computing
22 April – 03 May 2024 · Kathmandu, Nepal

Cell Project: My First Attempt at Parallelization

Motivation for ICTP School

communications biology

ARTICLE

https://doi.org/10.1038/s42003-022-03174-6 OPEN

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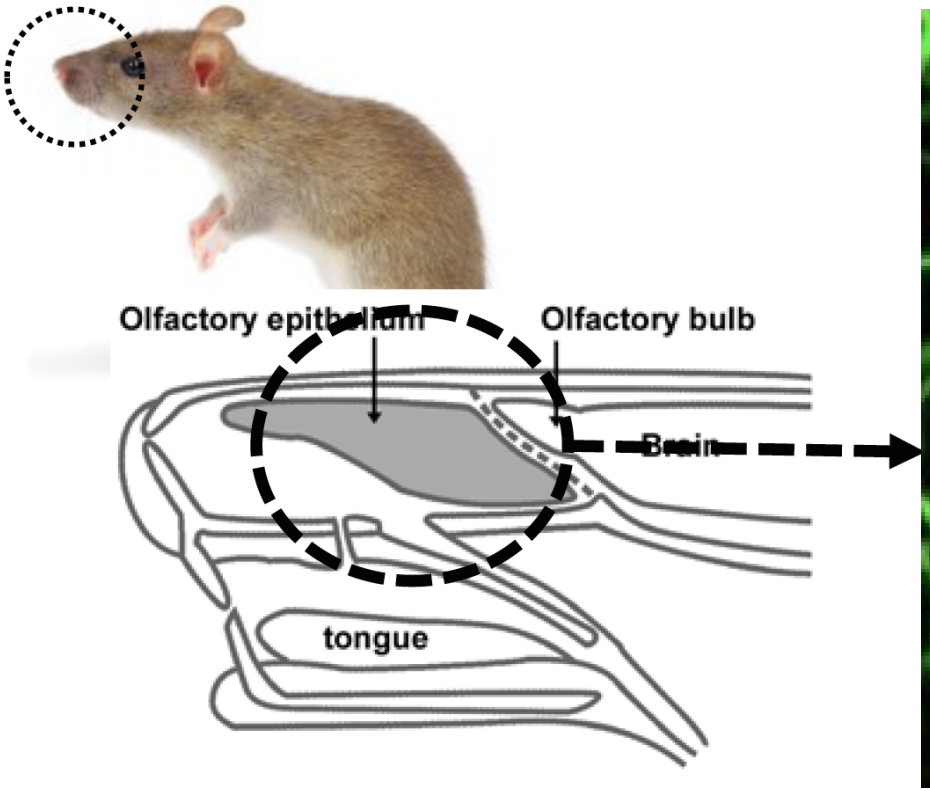
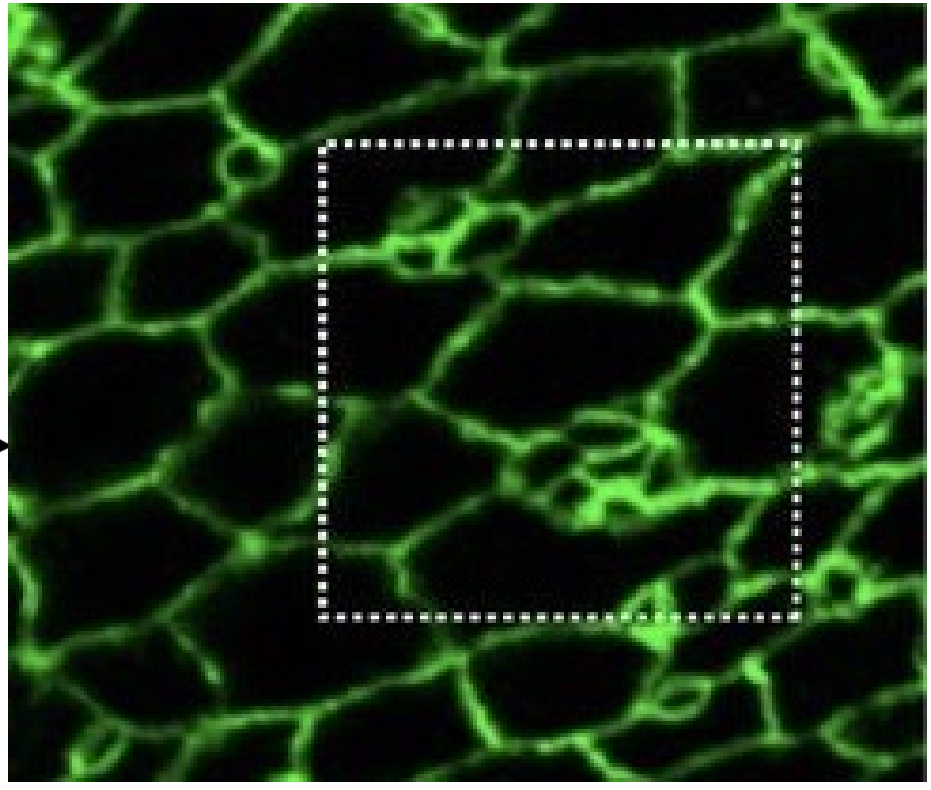
A numerical algorithm for modeling cellular rearrangements in tissue morphogenesis

Rhudaina Z. Mohammad [1,2], Hideki Murakawa [3], Karel Svadlenka [1,4✉] & Hideru Togashi [5,6]

- computational framework based on a level set formulation for tissue morphogenesis
- investigated cellular patterns observed in embryonic auditory and olfactory epithelium

Cellular Patterns in Sensory Epithelium





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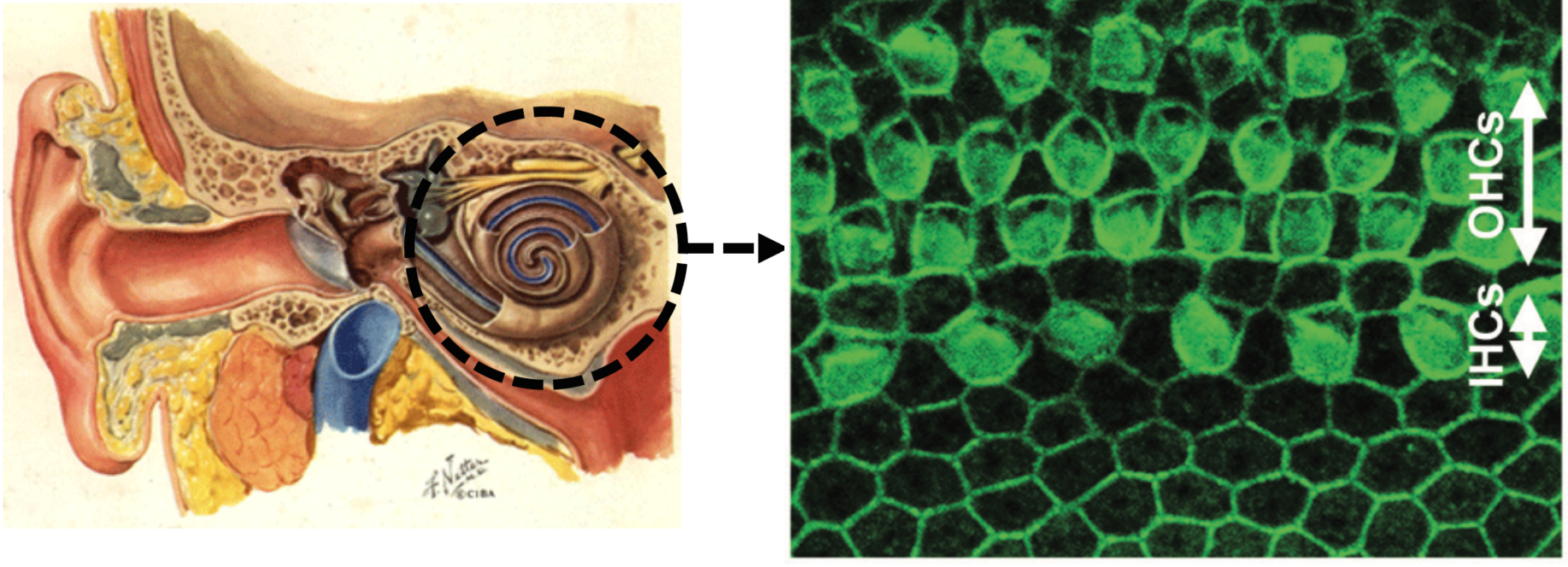
Cellular patterning in the olfactory epithelium (OE), located inside the nasal cavity of a wild-type mouse at embryonic day 14

Cellular Patterns in Sensory Epithelium



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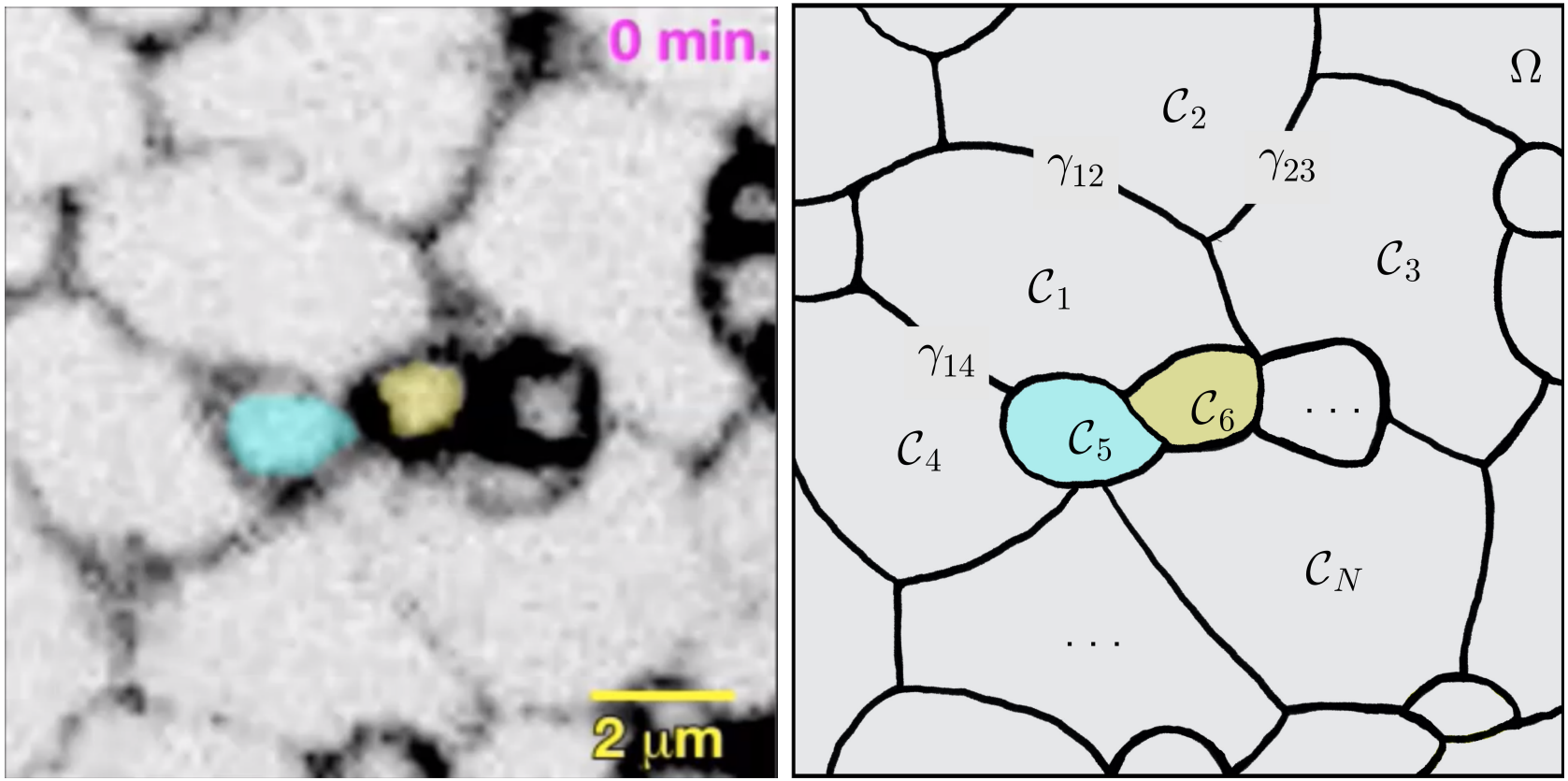
Cellular patterning in the auditory epithelium (AE), located in the cochlea of a wild-type mouse at postnatal day 1

Cellular Patterns in Sensory Epithelium

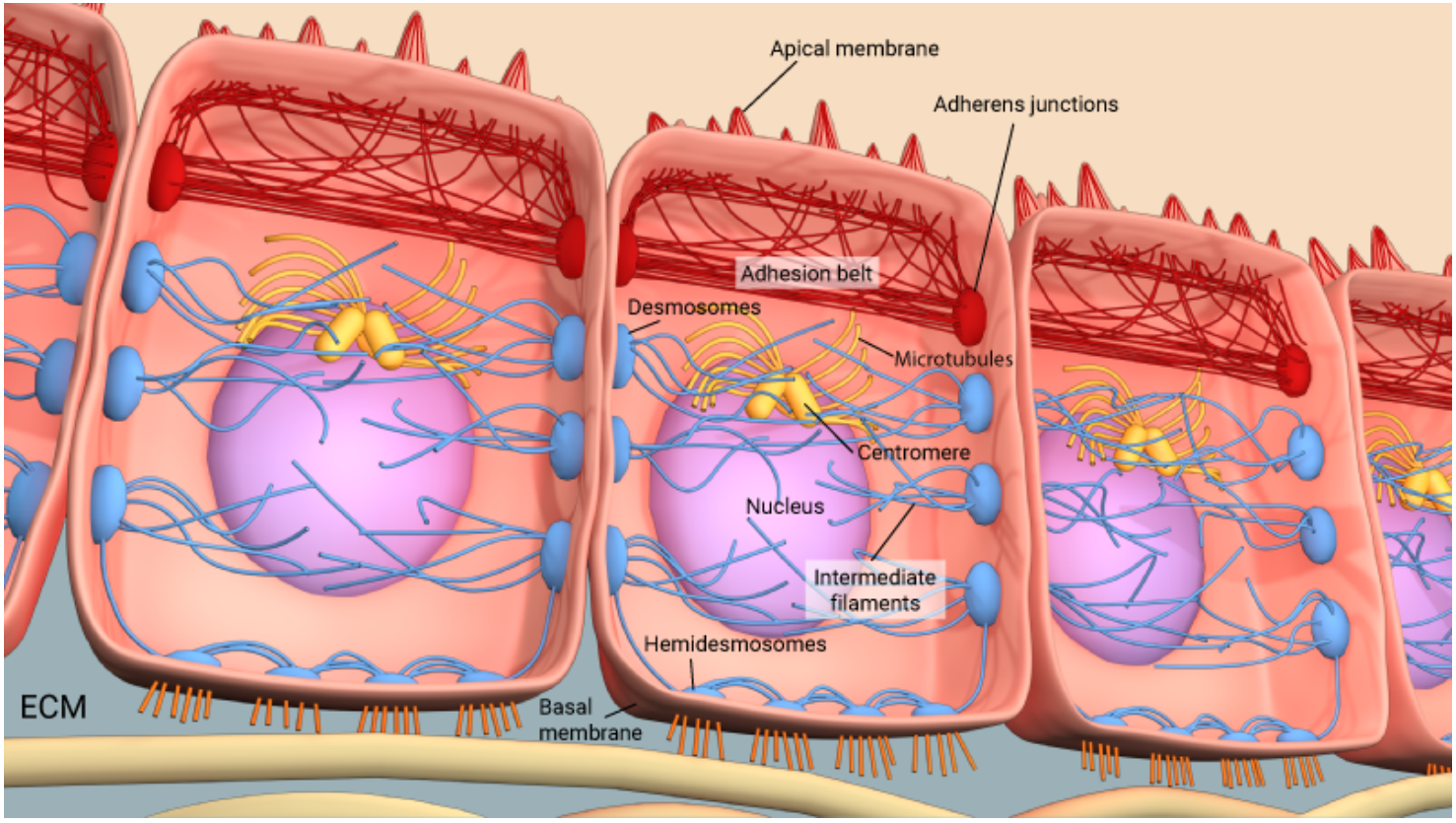
To analyze the effect of these factors in tissue morphogenesis, we assume

- tissue evolves via a succession of quasi-equilibrium states, i.e, cell shapes are described by their instantaneous state of lowest energy
- no apoptosis occurs during the evolution



Microscopy image of mouse OE culture prepared at E14 [Katsunuma et al., 2016] and its schematic diagram. OCs are indicated by blue and yellow.

Cellular Patterns in Sensory Epithelium



Retrieved from https://www.mechanobio.info/epithelial-cells-junctions-2/

Epithelial cell-cell adhesions are mediated via adherens junctions (AJs), where nectins and cadherins cooperate and bind the intracellular proteins p120-catenin and β-catenin

Cellular Patterns in Sensory Epithelium

Consider an aggregate of cells as a bounded domain

$$\Omega = \mathcal{C}_1 \cup \cdots \cup \mathcal{C}_N \subset \mathbb{R}^d$$

partitioned into N cells where cell-cell junction

$$\gamma_{ij} := \mathcal{C}_i \cap \mathcal{C}_j = \partial\mathcal{C}_i \cap \partial\mathcal{C}_j$$

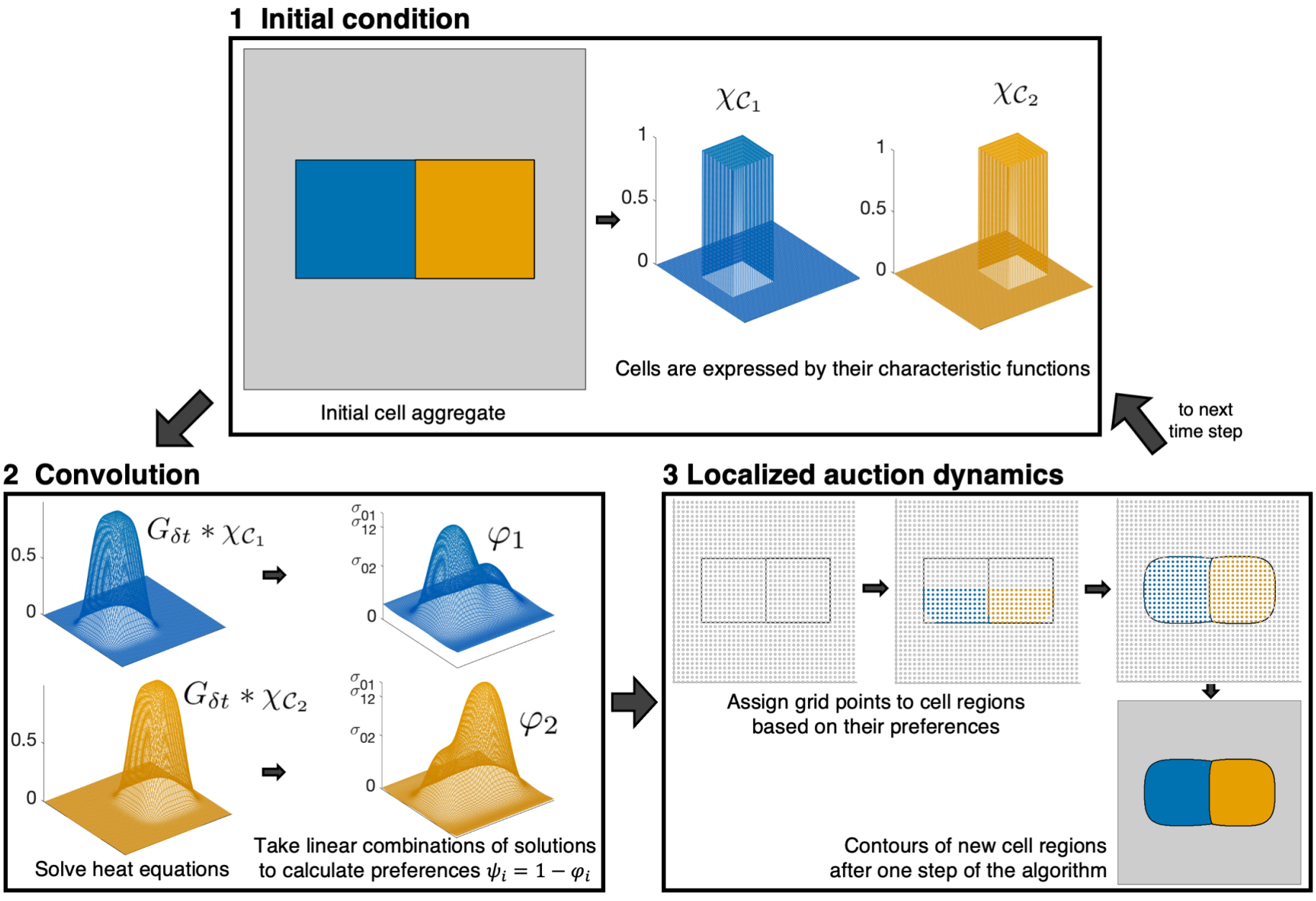
Take cellular rearrangement as L^2-gradient flow of a weighted surface energy

$$E(\mathcal{C}_1, \ldots, \mathcal{C}_N) = \sum_{i \neq j} \sigma_{ij} \int_{\gamma_{ij}} d\mathcal{H}^{d-1},$$

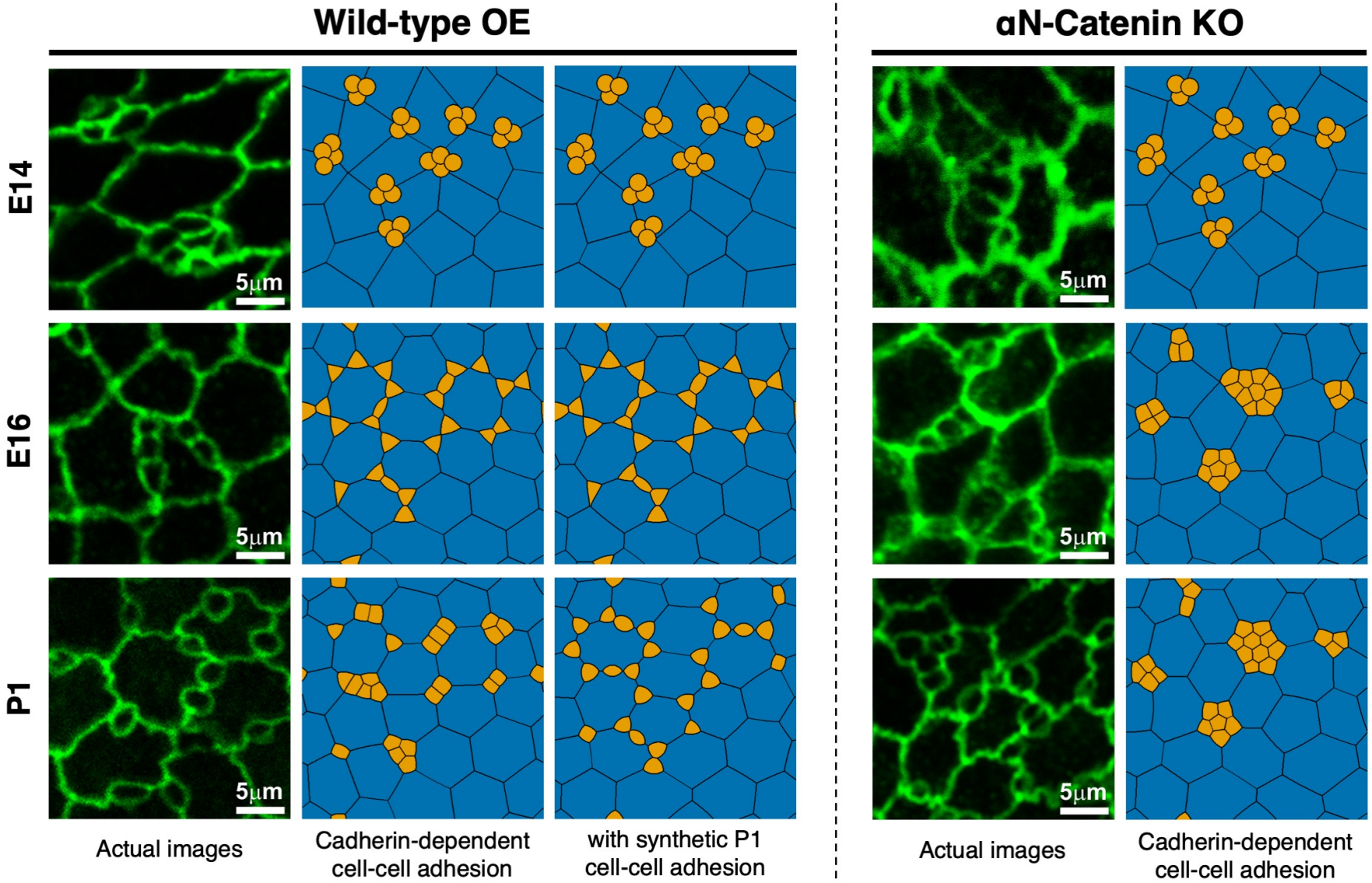
constrained by each cell's prescribed volume V_k^0 $(k = 1, 2, \ldots, N)$.

- Here, σ_{ij}'s are derived from measured values such as cell-cell adhesion (interfacial tension).

Proposed Algorithm

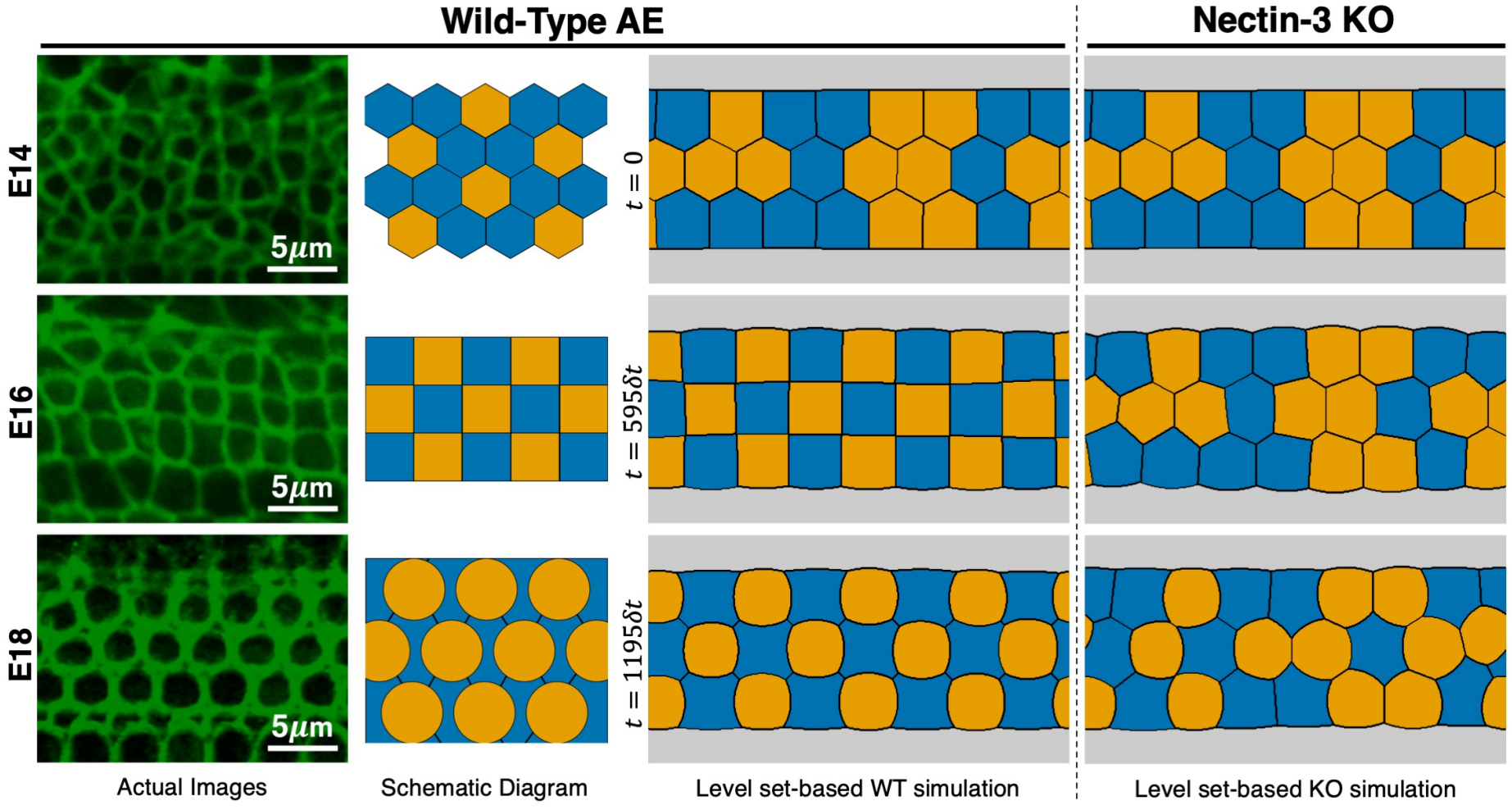


Developing OE Simulation



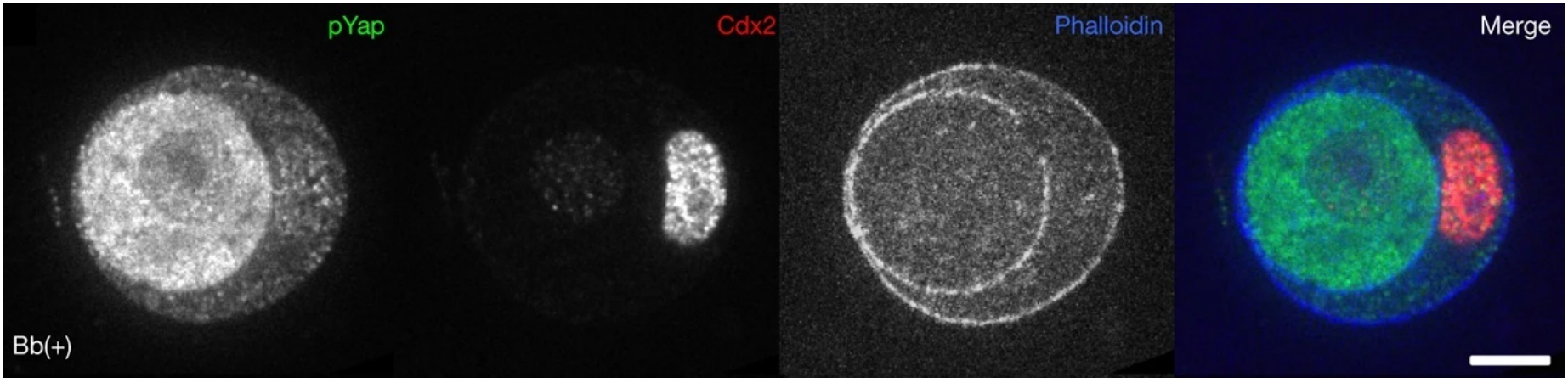
[Katsunuma et al., 2016]: during development, olfactory cells (OCs) and supporting cells (SCs) dynamically arrange themselves to form a mosaic

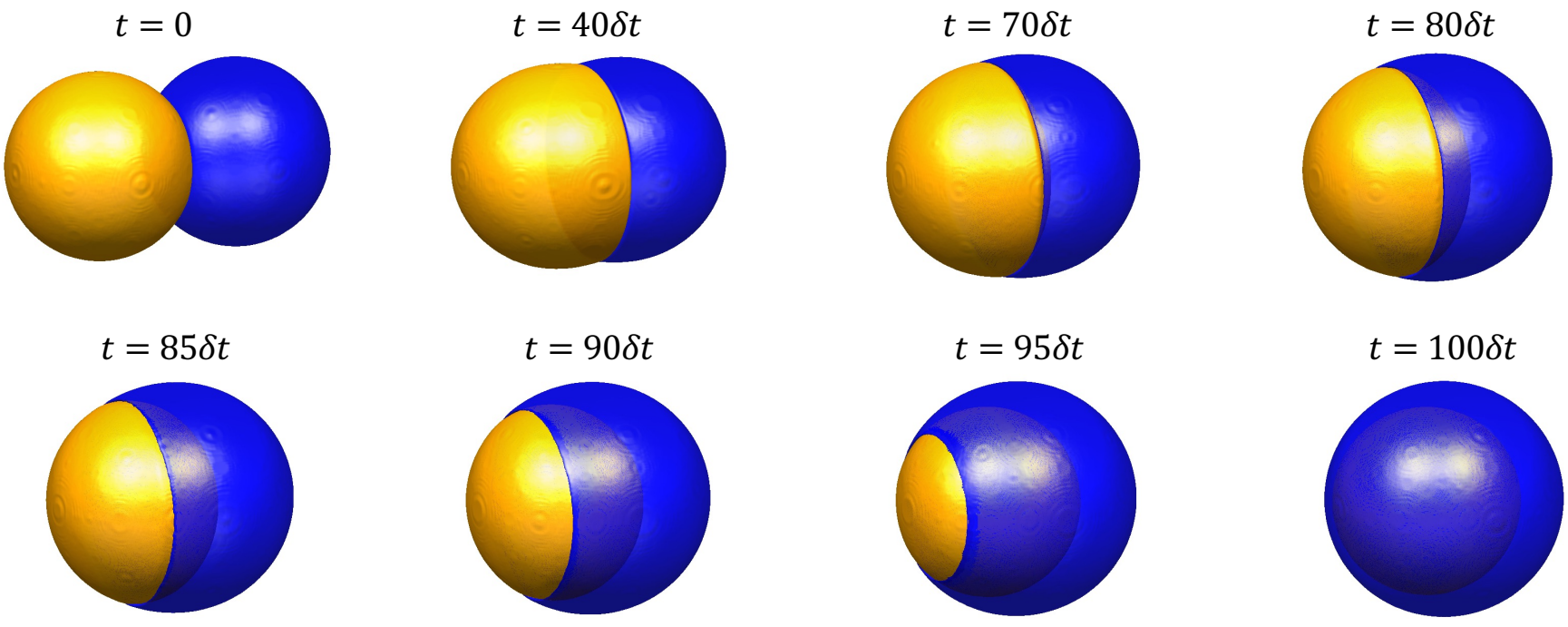
Developing AE Simulation



[Togashi 2016]: cellular rearrangement of AE from embryonic day 14 to 18

Embryo Morphogenesis

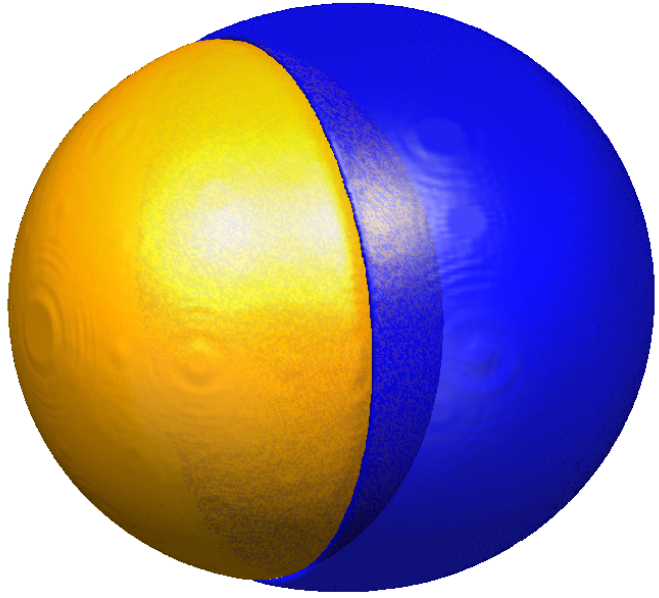




[Maitre et al. 2016]: embryo morphogenesis reveals that cells internalize only when differences in surface contractility exceed a predictable threshold

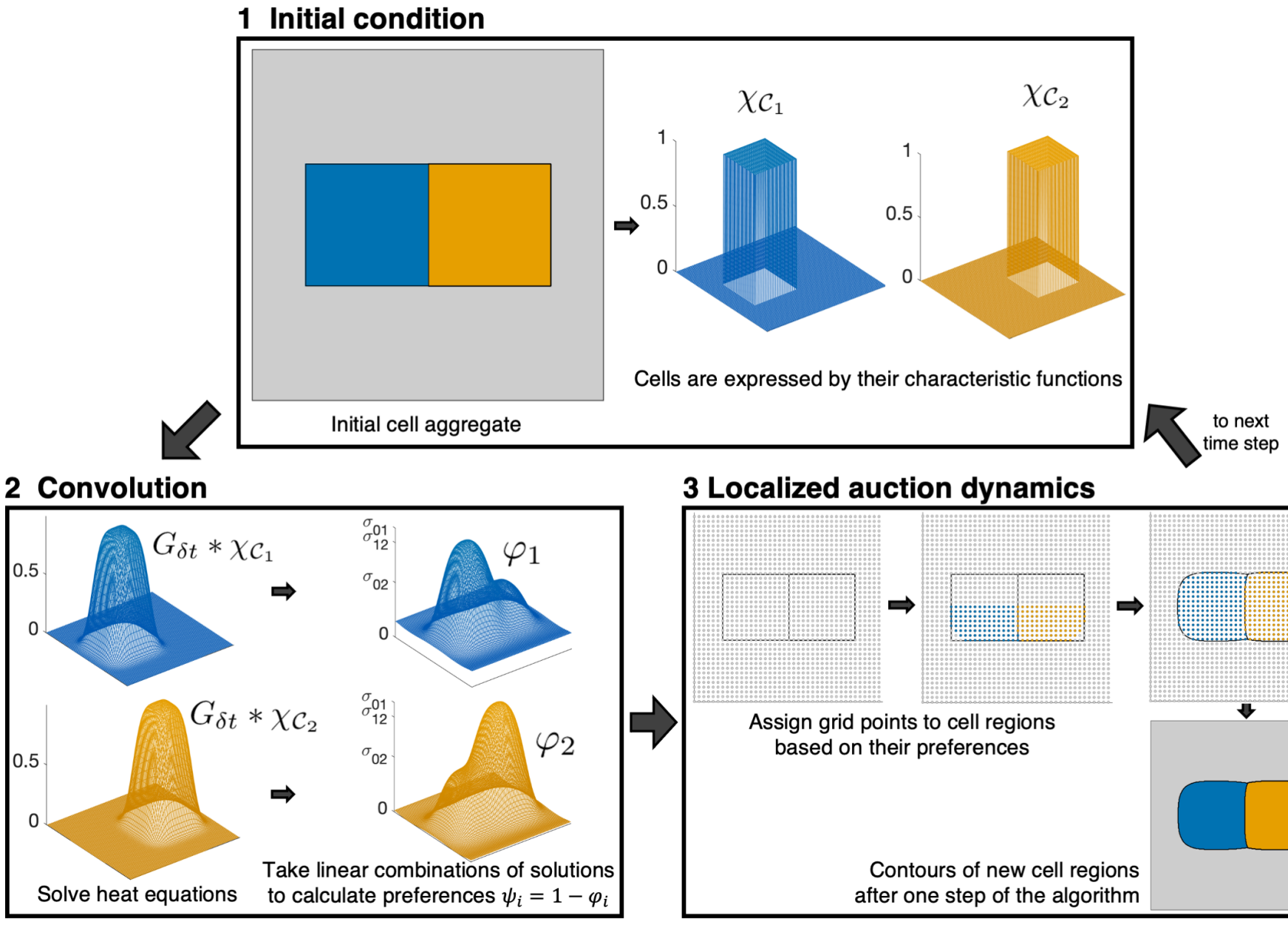
Embryo Morphogenesis

Level Set-based Scheme: **t = 0.400000**



$\sigma_{BB} = 1.00$ $\sigma_{BO} = 0.50$ $\sigma_{OO} = 1.00$ $\sigma_{BW} = 1.00$ $\sigma_{OW} = 1.36$ $\sigma_{WW} = 1.00$

Attempt at Computational Acceleration

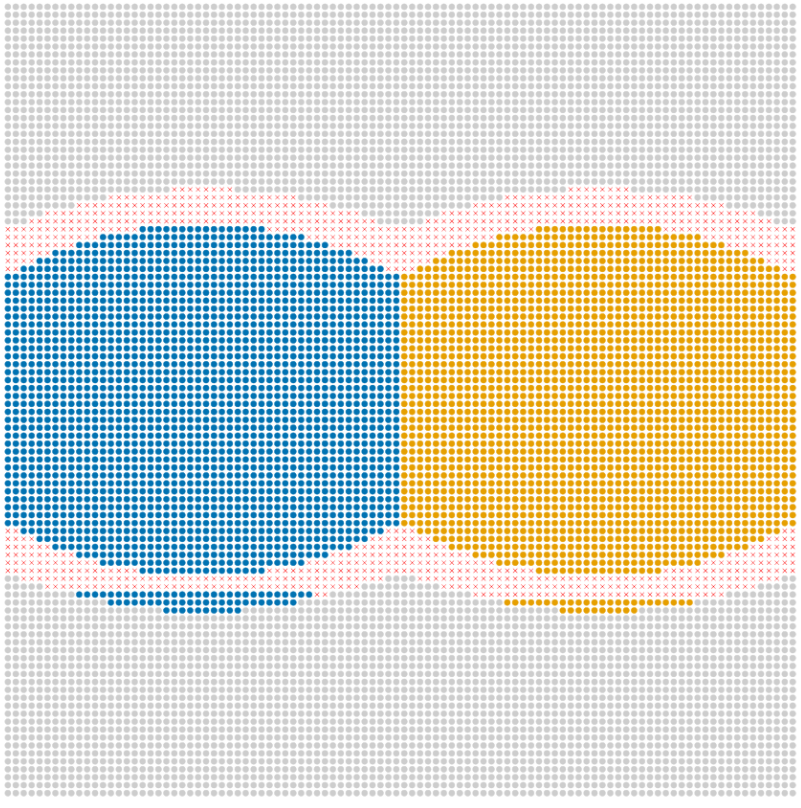


Attempt at Computational Acceleration

```
    // Define FFTW plans
    int nthreads = 1;
#if defined(_OPENMP)
    nthreads = omp_get_max_threads();
    printf("Running FFTW %d OpenMP threads...\n", nthreads);
#endif
    int normCoef = nbCells*nbNodes;
    int nbCmplxNodes = ((int)(nbNodesByCol/2)+1)*nbNodesByRow;
    if (dim==3) nbCmplxNodes *= nbNodesByRow;
    int *nbPerDim = (int *) malloc((dim+1)*sizeof(int));
    for (int i = 1; i < dim+1; i++) nbPerDim[i] = nbNodesByRow;
    nbPerDim[0] = nbCells;
    if (dim==2) nbPerDim[2] = nbNodesByCol;

    double freqStepX = (nbNodesByCol-1.)/nbNodesByCol;
    double freqStepY = (nbNodesByCol-1.)/nbNodesByRow;

#if defined(_OPENMP)
    int status = fftw_init_threads();
    if (status==0){
      printf("FFTW error in thread initialization.\n");
    }
    fftw_plan_with_nthreads(nthreads);
#endif
    fftw_complex *ft_phi = fftw_malloc(nbCells*nbCmplxNodes*sizeof(fftw_complex));
    fftw_plan forward;
    if (dim==2) forward = fftw_plan_dft_r2c_3d(nbCells, nbNodesByRow, nbNodesByCol, phi, ft_phi, FFTW_MEASURE);
    if (dim==3) forward = fftw_plan_dft_r2c(4, nbPerDim, phi, ft_phi, FFTW_MEASURE);
    fftw_plan backward;
    if (dim==2) backward = fftw_plan_dft_c2r_3d(nbCells, nbNodesByRow, nbNodesByCol, ft_phi, phi, FFTW_MEASURE);
    if (dim==3) backward = fftw_plan_dft_c2r(4, nbPerDim, ft_phi, phi, FFTW_MEASURE);

    // Export initial configuration to output
    export_solution(0, nbNodes, isAssigned);
    display_data(dim, nbNodes, nbCells, nbTypes, dt, typeTension);
```

Auction Dynamics

Auction Dynamics



assigned nodes: 09098/10000

node: 2539

preferred cell : C_1

bid on C_1: 0.02032

*assign to C_1

Cell volume

C_0(gray) : 5000/5000

C_1(blue) : 2064/2500

C_2(orange) : 2034/2500

Cell price

p_0: 0.14838

p_1: 0.00000

p_2: 0.00000

Jacobi Algorithm for Solving Laplace Equation

Jacobi Algorithm

Consider the Laplace equation:

$$\begin{cases} \Delta u = 0, & \text{in } [a,b]^2 \\ u = 0, & \text{on } \{x=b\} \cup \{y=b\} \\ u = -\frac{100}{b-a}(y-a) + 100, & \text{on } \{x=a\} \\ u = -\frac{100}{b-a}(x-a) + 100, & \text{on } \{y=a\} \end{cases}$$

Jacobi Algorithm

- Discretize the domain into $(n+2)^2$ points (x_i, y_j) where

$$a = x_0 < x_1 < \cdots < x_n < x_{n+1} = b$$

$$a = y_0 < y_1 < \cdots < y_n < y_{n+1} = b$$

- On a regular grid, we can approximate the Laplacian

$$\Delta u = u_{xx} + u_{yy}$$

using central difference method

$$u_{xx}(x,y) \approx \frac{u(x+h,y) - 2u(x,y) + u(x-h,y)}{h^2}$$

and

$$u_{yy}(x,y) \approx \frac{u(x,y+h) - 2u(x,y) + u(x,y-h)}{h^2}$$

Jacobi Algorithm

- Denoting $u_{i,j} = u(x_i, y_j)$, we get

$$\Delta u \approx \frac{u_{i+1,j} + u_{i-1,j} - 4u_{i,j} + u_{i,j+1} + u_{i,j-1}}{h^2}$$

- Since $\Delta u = 0$, we have

$$u_{i,j} \approx \frac{u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1}}{4}$$

- Starting from an initial guess u^0, we generate a sequence of approximate solutions

$$u_{i,j}^{k+1} = \frac{u_{i+1,j}^k + u_{i-1,j}^k + u_{i,j+1}^k + u_{i,j-1}^k}{4}, \quad k = 0, 1, 2 \ldots$$

  such that $u^k \to u$, the solution of the Laplace equation as $k \to \infty$.

Jacobi Algorithm: 1D Decomposition

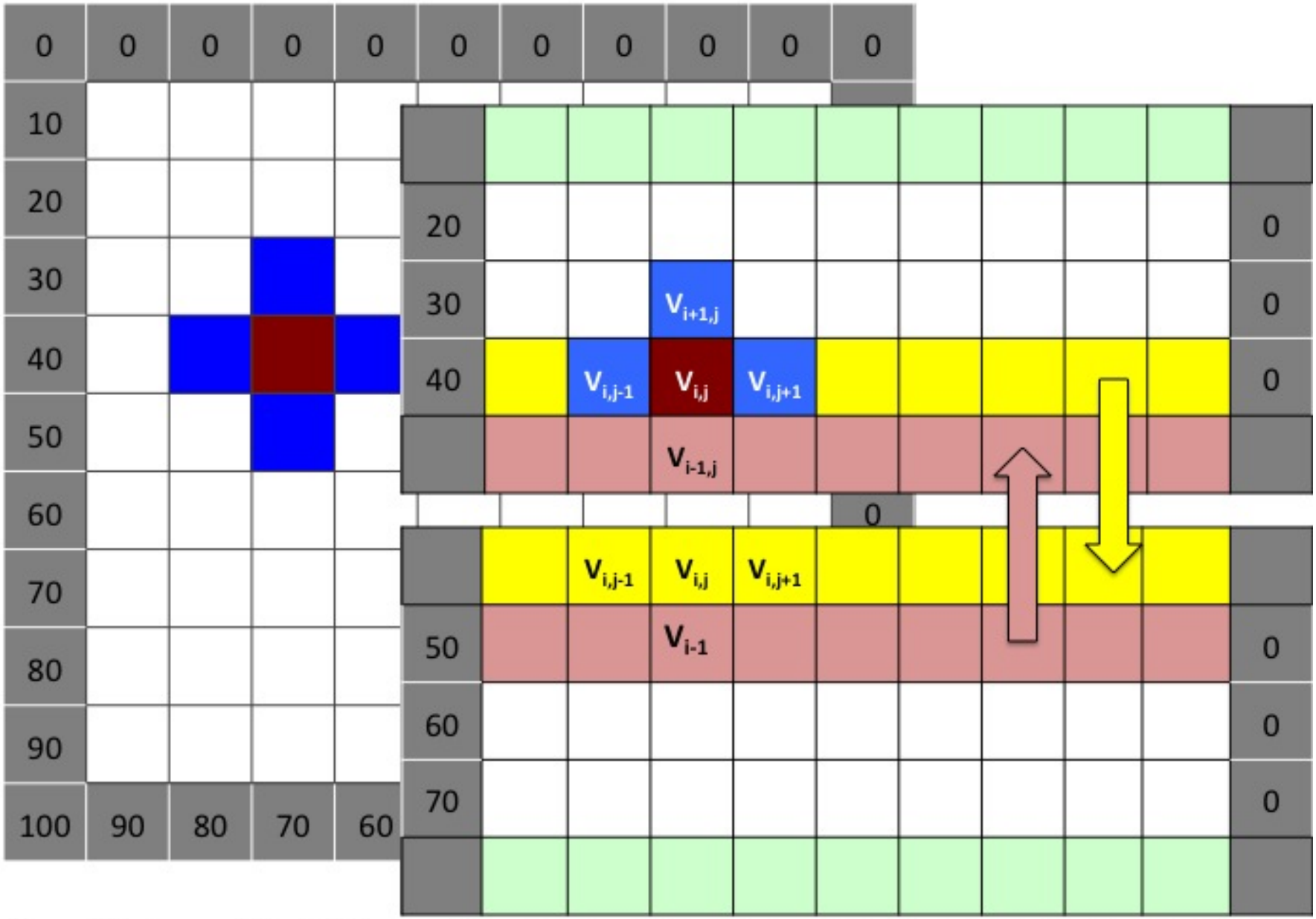


Figure 2: A diagram of the 1-D decomposition of the Jacobi Relaxation for Solving the Laplace's Equation, showing that the boundary elements that need to be communicated between processors.

Jacobi Algorithm: 1D Decomposition

```
int dim = atoi(argv[1]);
int max_iter = atoi(argv[2]);

int me, npes, n_loc, rest, offset=0;
MPI_Init( &argc, &argv );
MPI_Comm_rank( MPI_COMM_WORLD, &me );
MPI_Comm_size( MPI_COMM_WORLD, &npes );
MPI_Barrier(MPI_COMM_WORLD);  //synchronize all processes

double t_start, t_end, t_elapsed;
t_start = MPI_Wtime();

n_loc = dim/npes + 2;
rest = dim % npes;
if( me < rest ) n_loc += 1;
else offset = rest;

double* matrix = NULL;
matrix = (double *)  malloc(sizeof(double) * dim * n_loc);
if (matrix == NULL){
  printf("[ERROR] Check memory allocation for the matrix.\n");
  exit(-1);
}
memset(matrix, 0.5, sizeof(double) * dim * n_loc);
```

Jacobi Algorithm: 1D Decomposition

```
void communicate(double *matrix, int n_loc, int dim, int npes, int me){
  // Send up and send down
  if(me != 0){
    // send up the 2nd row (idx = 1) of previous processor (tag = 1)
    MPI_Send(matrix + dim, dim, MPI_DOUBLE, me-1, 1, MPI_COMM_WORLD);
  }
  if(me!= npes-1){
    // send down the second-to-the-last row (idx = n_loc-2) of next processor (tag = 2)
    MPI_Send(matrix + (n_loc-2)*dim, dim, MPI_DOUBLE, me+1, 2, MPI_COMM_WORLD);
  }

  // Receive from above and and from below
  if(me!= 0){
    // receive from above and update 1st row (tag = 2)
    MPI_Recv(matrix, dim, MPI_DOUBLE, me-1, 2, MPI_COMM_WORLD, MPI_STATUS_IGNORE);
  }
  if(me!= npes-1){
    // receive from below and update last row (tag = 1)
    MPI_Recv(matrix + (n_loc-1)*dim, dim, MPI_DOUBLE, me+1, 1, MPI_COMM_WORLD, MPI_STATUS_IGNORE);
  }
}
```

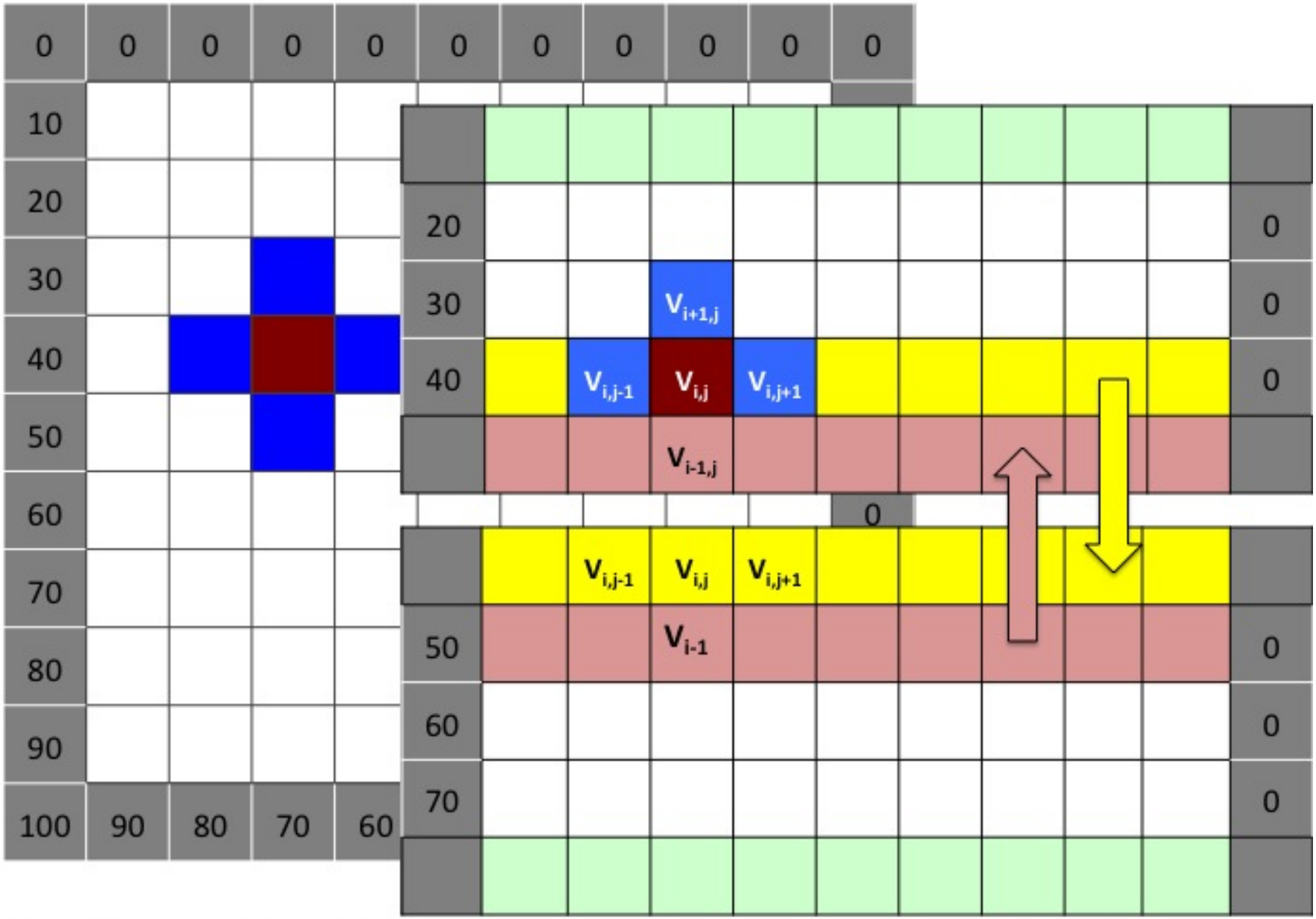
Jacobi Algorithm: 1D Decomposition

```
double err_chunk = 0;
for (int i = 1; i < n_loc-1; i++){
  for(int j = 0; j < dim; j++){
    // stencil west
    if (j == 0) west = (me*(n_loc-2) + i + offset) * increment;
    else        west = matrix[i*dim + j-1];
    // stencil east
    if (j == dim-1) east = 0;
    else            east = matrix[i*dim + j+1];

    new_mat[i*dim + j] = 0.25*( matrix[(i-1)*dim + j] + matrix[(i+1)*dim + j]
    + west + east );

    err_chunk += pow(new_mat[i*dim +j] - matrix[i*dim +j], 2);
  }
}
```

Jacobi Algorithm: 1D Decomposition

```
double west, east;
double increment = 100.0 / (dim+1);
for (size_t it = 0; it < max_iter; it++) {
  double err_chunk = 0;
  for (int i = 1; i < n_loc-1; i++){

  // Replace matrix values by new_mat values
  for (int i=1; i < n_loc-1; i++){
    for(int j=0; j < dim; j++){
      matrix[i*(dim) + j] = new_mat[i*(dim) + j ];
    }
  }
  communicate(matrix, n_loc, dim, npes, me);

  double error = 0;
  MPI_Allreduce(&err_chunk, &error, 1, MPI_DOUBLE, MPI_SUM, MPI_COMM_WORLD);
  if (me == 0) {
    printf("it %zu:\t %.7f\n", it, sqrt(error) );
    fprintf(file, "%.7f\n", sqrt(error) );
    if (sqrt(error) < TOL) break;
  }
}
```

Jacobi Algorithm: 1D Decomposition



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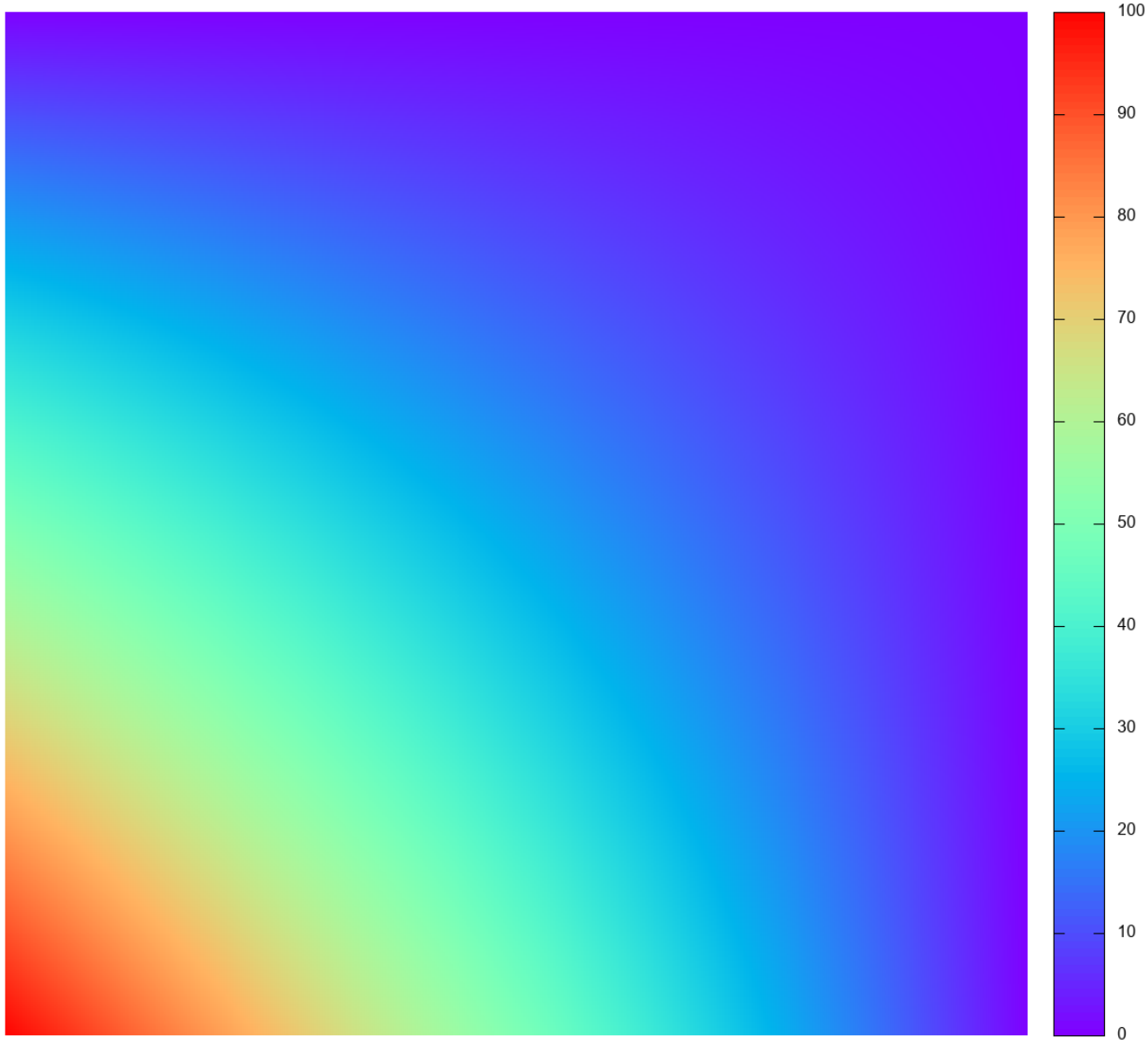
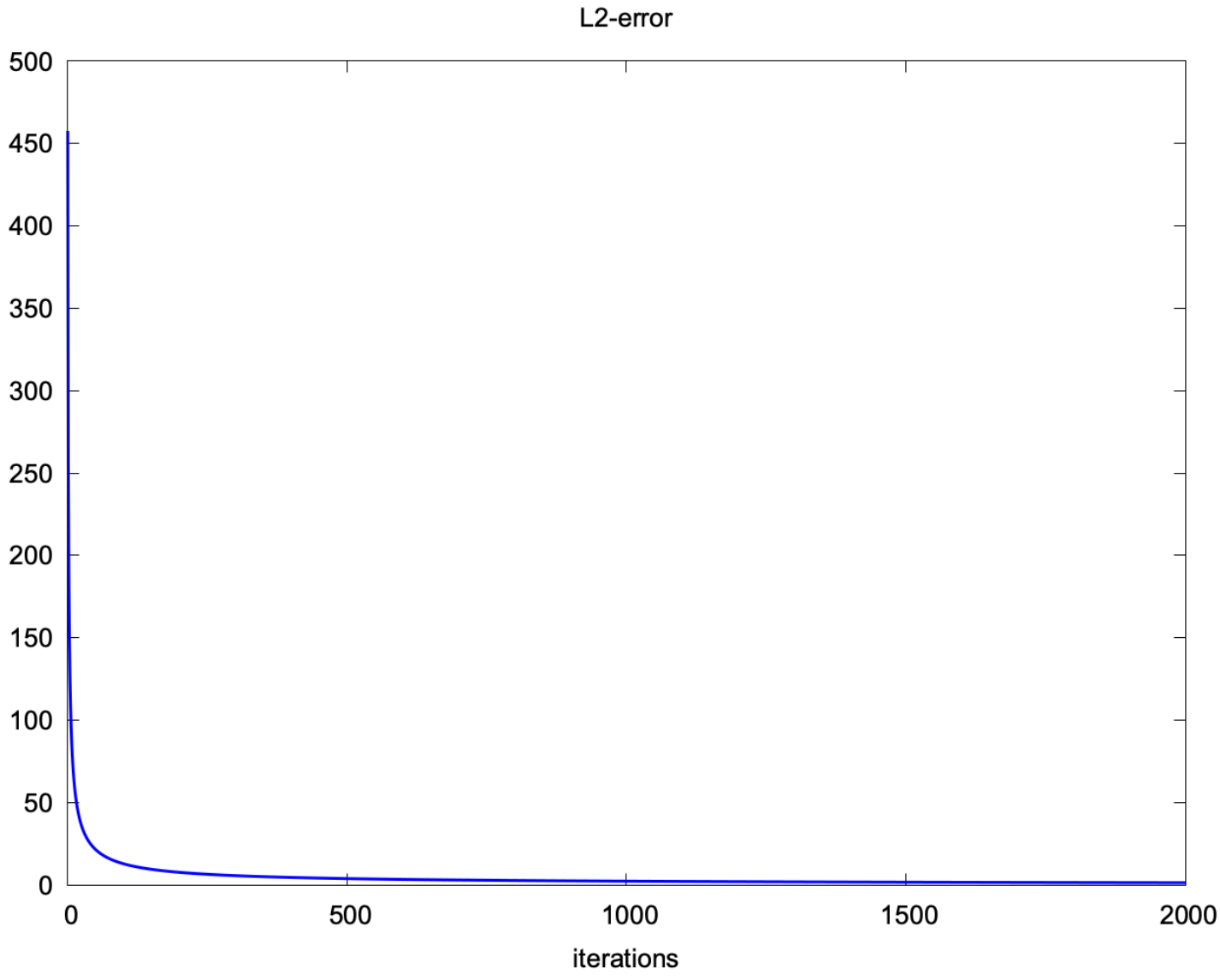
Jacobi Algorithm: 1D Decomposition



Jacobi Algorithm: 1D Decomposition



Thank you!