Highly Programmable Matter & Generalized Computation

Research in Reconfigurable Analog & Digital Computation In Bulk Materials

Bruce J. MacLennan Dept. of Computer Science University of Tennessee, Knoxville

"Radical Reconfiguration"

- Ordinary reconfiguration changes connections among fixed components
- Radical reconfiguration of <u>transducers</u>

to create new sensors & actuators

- Radical reconfiguration of processors
 - to reallocate matter to different components
- Also for repair & damage recovery
- Requires rearrangement of atoms and molecules into new components
- Requires "molar parallelism"

14 Feb. 2007

Our Ongoing Research in Radical Reconfiguration

- Programmable matter
 - Computational control of matter
 - Molecular combinatory computing
 - Morphogenetic approaches
- Generalized computation
 - Flexible general computing medium
 - Encompassing both analog & digital
 - U-machine

Molecular Combinatory Computing

- Comb. comp. based on two graph substitutions
 - computationally universal
 - can compile programs into these computational graphs
- Can proceed asynchronously & in parallel
- Program computes into structure represented in molecules
- Supported by NSF (Nanoscale Exploratory Research)



Morphogenetic Approaches



- Based on models of embryological development
- Cells migrate by local interaction & chemical signals
- Possible implementation: "programmable" micro-organisms

Computation in General Sense

- A definition applicable to computation in nature as well as computers
- Computation is a *physical* process, the purpose of which is *abstract* operation on *abstract* objects
- A computation must be implemented by *some* physical system, but it may be implemented by *any* physical system with the appropriate abstract structure

Abstract Spaces

- Should be general enough to include continuous & discrete spaces
- Hypothesis: *separable metric spaces*
- Include continua & countable discrete spaces
- separable \Rightarrow approximating sequences

The U-Machine

- Goal: a model of computation over abstract spaces that can be implemented in a variety of physical media
- In particular, bulk nanostructured materials in which:
 - access to interior is limited
 - detailed control of structure is difficult
 - structural defects and other imperfections are unavoidable

Urysohn Embedding

- A separable metric space is homeomorphic to a subset of a Hilbert space
- Let (X, δ) be separable metric space
- Let $b_1, b_2, \ldots \in X$ be a ctbl dense subset
- WLOG suppose δ is bounded in [0, 1]
- Let similarity $\sigma(x, y) = 1 \delta(x, y)$
- Define:

$$U(x) = \left(\frac{\sigma(x,b_1)}{1}, \frac{\sigma(x,b_2)}{2}, \frac{\sigma(x,b_3)}{3}, \dots\right)$$

Urysohn Embedding







Field Computation

- Field = continuous distribution of continuous quantity = element of Hilbert function space
- u_k used to scale basis functions
- Linear superposition represents element of abstract space





An Abstract Cortex

- Finite-dimensional representations of abstract spaces can be allocated disjoint regions in data space
- Field representations can be allocated to separated regions
- Analogous to regions in neural cortex



Decomposition of Computations

- Complex computations may be decomposed into simpler ones
- Variable regions provide interfaces between constituent computational processes
- For "radical reconfiguration": don't build in specific primitive processes
- How are primitive processes implemented?

Implementation of Primitive Computations

There are several "universal approximation theorems" that make use of approximations of the form:

$$\mathbf{v} = \mathbf{F}(\mathbf{u}) \approx \sum_{j=1}^{\infty} \vec{\alpha}^{j} r_{j}(\mathbf{u})$$

Works for a variety of simple nonlinear
 "basis functions" r_j

Example Interpolation Method

- Training samples: $(x_1, y_1), ..., (x_P, y_P)$
- Hilbert space reprs.: $\mathbf{u}^k = U(x_k), \mathbf{v}^k = V(y_k)$
- Interpolation conditions: $\mathbf{v}^k = \sum_j \vec{\alpha}^j r_j (\mathbf{u}^k)$

• Let
$$V_{ki} = v_i^k$$
, $R_{kj} = r_j(\mathbf{u}^k)$, $A_{ji} = \alpha_i^j$

- Exact interpolation: V = RA
- Best (least squares) approx.: $\mathbf{A} \approx \mathbf{R}^+ \mathbf{V}$ where $\mathbf{R}^+ = (\mathbf{R}^T \mathbf{R})^{-1} \mathbf{R}^T$

Typical Basis Functions

- Perceptron-style: $r_j(\mathbf{u}) = r(\mathbf{w}_j \cdot \mathbf{u} + b_j)$
- Radial-basis functions:

$$r_j(\mathbf{u}) = r\left(\left\|\mathbf{u} - \mathbf{c}_j\right\|\right)$$

- Green's function for stabilizer: $r_j(\mathbf{u}) = G(\mathbf{u}, \mathbf{u}^j)$
- Key point: <u>lots of choices</u>

Determination of Interconnection Matrices

- Unknown functions: neural-net training
- Known function compute offline by:
 - Generating sufficient interpolation samples, or:
 - Determining matrices analytically
- Typical primitives could include those found typically on analog or digital computers

Merging Linear Transforms

- General form of approximation: $\mathbf{v} = \mathbf{A} \mathbf{r}(\mathbf{B}\mathbf{u})$, where $[\mathbf{r}(\mathbf{B}\mathbf{u})]_j = r([\mathbf{B}\mathbf{u}]_j)$
- Suppose: $\mathbf{w} = \mathbf{A}' \mathbf{r}'(\mathbf{B}'\mathbf{v})$
- Linear parts can be combined:
 w = A' r'[C r(Bu)], where C = B'A
- Two basic operations:
 - Matrix-vector multiplication
 - Simple point-wise nonlinear function \mathbf{r}

Input Transduction

- Input space: (X, δ)
- Suitable ϵ -net: $(b_1, b_2, ..., b_n)$
- Hilbert-space representation $\mathbf{u} = U(x)$: $u_k = \sigma (x, b_k),$ where $\sigma (x, b_k) = 1 - \delta (x, b_k)$
- In effect have fuzzy feature detectors: $\sigma_k(x) = \sigma(x, b_k)$
- Thus $\mathbf{u} = (\sigma_1(x), \sigma_2(x), ..., \sigma_n(x))^T$

Output Transduction

- Physical output spaces are usually vector spaces
- Approximate by: $y = V^{-1}(\mathbf{v}) \approx \sum_{j=1}^{n} \mathbf{a}^{j} r_{j}(\mathbf{v})$
- This summation is a physical superposition of physical vectors aⁱ
- Compute approximation parameters in any of the usual ways

Real-time Computation

- Time-varying input & outputs *x*(*t*) are represented by time varying vectors **u**(*t*)
- Differential changes are computed like other functions
- Differential changes are integrated into variable regions

(Re-)Configuration Methods

Overall Structure

- Variable (data) space
 - Large number of scalar variables for Hilbert coefficients
 - Partitioned into regions representing abstract spaces
- Function (program) space
 - Flexible interconnection (.:. 3D)
 - Programmable linear combinations
 - Application of basis functions

Depiction of UM Interior



- Shell contains variable areas & computational elements
- Interior filled with solid or liquid *matrix* (not shown)
- Paths formed through or from matrix

Layers in Data Space



- Connection matrix has programmable weights
- Linear combinations are inputs to nonlinear basis functions
- Exterior access to both sides for programming

Depiction of UM Exterior



Diffusion-Based Path Routing



Example Path-Routing Process

- Attractant diffuses from destination
 - Could be chemical, electrons, molecular state
 - Attractant degrades
- Existing paths clamp attractant to 0
 - Effectively repel new path
- Path "grows" from source by climbing attractant gradient
 - Attractant injection rate ramped up
- After connection made, attractant allowed to decay before routing next path

Example of Path Routing



- Starts and ends chosen randomly
- Quiescent interval (for attractant decay) omitted from video
- Each path occupies ~0.1% of space
- Total: ~4%

Front



Right



Back



Left



Тор



Bottom



Remarks

- More realistic procedure:
 - Systematic placement of regions
 - Order of path growth
 - Control of diffusion & growth phases
- General approach is robust (many variations work about as well)
- Paths could be formed by:
 - Migration of molecules etc.
 - Change of state of immobile molecules

Example Connection-Growth Process

- Goal: approximately full interconnection between incoming "axons" (A) and "dendrites" (D) of basis functions
 - Doesn't have to be perfect
- Each A & D periodically initiates fiber growth
 - Growth is approximately away from source
- Fibers repel others of same kind
 - Diffusible, degradable repellant
 - Fibers follow decreasing gradient (in XZ plane)
- Contact formed when A and D fibers meet

Example of Connection Formation



- 10 random "axons" (red) and "dendrites" (blue)
- Simulation stopped after 100 connections (yellow) formed

Resulting Connections



Setting Connection Strengths by SVD

• Let $m \times n$ connection matrix $\mathbf{M} = \mathbf{U} \Sigma \mathbf{V}^{\mathrm{T}}$, where $\Sigma = \begin{bmatrix} \Sigma_r & 0 \\ 0 & 0 \end{bmatrix}$

and $\Sigma_r = \text{diag}(s_1, \ldots, s_r)$

- Let \mathbf{u}_k and \mathbf{v}_k be columns of \mathbf{U} and \mathbf{V} : $\mathbf{U} = [\mathbf{u}_1, ..., \mathbf{u}_m], \mathbf{V} = [\mathbf{v}_1, ..., \mathbf{v}_n]$
- Then,

$$\mathbf{M} = \sum_{k=1}^{r} s_k \mathbf{u}_k \mathbf{v}_k^{\mathrm{T}}$$

• For each *k*, apply **v**_k to input and **u**_k to output and program with strength *s*_k

Summary of U-Machine

- Permits computation on quite general abstract spaces (separable metric spaces)
 - Includes analog & digital computation
- Computation by linear combinations & simple nonlinear basis functions
- Simple computational medium can be reconfigured for different computations
- Potentially implementable in a variety of materials

Computational Control of Matter

- A material process may be used as a substrate for formal computation
- Formal computation may be used to control a material process
- A material process may be a substrate for universal computation, controlled by a formal program
- A formal program may be used to govern a material process

The Physical State as Synthetic Medium

- Computation controls physical state (as synthesis medium)
- Reconfigured computer is embodied in physical state
- Computation must be able to distinguish synthetically relevant physical states

Universal Computer



Highly Programmable Matter







Equilibrium vs. Stationary Configurations

- Program terminates for equilibrium config.
- Program continues to run for stationary config.



Thermodynamics of a Configuration

- Either, configuration is a <u>stable state</u>
 - damage may shift to undesirable equilibrium
- Or, configuration is a <u>stationary state</u> of a non-equilibrium system
 - continuously reconfigures self
 - self-repair as return to original stationary state
 - adaptation & damage recovery as move to different stationary state

Useful Media for Computational Synthesis

- For pure computation, move as little matter & energy as possible
- For synthesis, need to control atoms & molecules as well as electrons
- Need sufficiently wide variety of controllable atoms & molecules
- Goal: structures on the order of optical wavelengths (100s of nm)

Models of Computation for Synthesis

- Need massive parallelism to control detailed organization of state
- Need tolerance to errors in state
 - synthesis program should be tolerant
 - configured computer should be tolerant

Locus of Control of Detailed Organization

- Reorganizing atoms & molecules
 ⇒ vast amount of detailed control
- Heterosynthesis
 - external configuration controller determines fine structure of medium (high bandwidth)
- Autosynthesis
 - external configuration controller determines general boundary conditions (low BW)
 - fine structure results from self-organization

General Model of Radical Reconfiguration

- Synthesis controller
 - low bandwidth to outside world
 - bandwidth to medium:
 - high for heterosynthesis
 - low for autosynthesis
- Synthetic medium
 - molar parallelism of interactions
 - simple for heterosynthesis
 - complex for autosynthesis
 - what are suitable synthetic media?

Example:

Activation-Inhibition System

- Let σ be the logistic sigmoid function
- Activator *A* and inhibitor *I* may diffuse at different rates in *x* and *y* directions
- Cell is "on" if activator + bias exceeds inhibitor

$$\frac{\partial A}{\partial t} = d_{Ax} \frac{\partial^2 A}{\partial x^2} + d_{Ay} \frac{\partial^2 A}{\partial y^2} + k_A \sigma \Big[m_A \big(A + B - I \big) \Big]$$
$$\frac{\partial I}{\partial t} = d_{Ix} \frac{\partial^2 I}{\partial x^2} + d_{Iy} \frac{\partial^2 I}{\partial y^2} + k_I \sigma \Big[m_I \big(A + B - I \big) \Big]$$

14 Feb. 2007

Double Activation-Inhibition System

- Two independently diffusing activation-inhibition pairs
- May have different diffusion rates in X and Y directions
 - In this example, $I_{1y} >> I_{1x}$ and $I_{2x} >> I_{2y}$
- Colors in simulation:
 - green = system 1 active
 - red = system 2 active
 - yellow = both active
 - black = neither active

Formation of Pattern



- Random initial state
- System stabilizes to < 1% cell changes
- Modest noise

 (annealing noise)
 improves regularity

Stationary State



- System is being continually maintained in a stationary state
- Continuing change < 1%

Recovery from Damage



- Simulated damage
- Damage destroys activators & inhibitors as well as structure
- System repairs self by returning to stationary state
- No explicit repair signal

Reconfiguration: Orthogonal Structure



- Exchange inhibitor diffusion rates for systems 1 & 2
- Vertical stripes become horizontal
- Horizontal stripes become vertical
- No explicit reconfiguration signal

Conclusions

- Radical reconfiguration can be accomplished by using computation to change matter
 - external control of macrostructure
 - self-organization of microstructure
- A simple, flexible architecture can compute over a variety of abstract spaces (including analog & digital)