

Systems Biology on Bio-Linux

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<http://nebc.nerc.ac.uk/tools/bio-linux>

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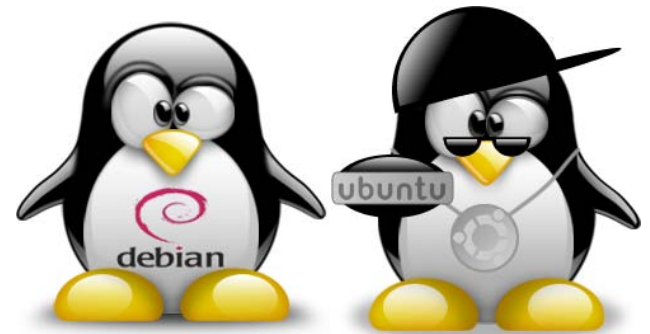
2. Modelling Approaches: Top-Down / Bottom-Up / Hybrid

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1. Bio-Linux: A Computational Biology Workstation

“one-stop-shop computational solution
-- from desktop to the cloud --
for biologists and bioinformaticians alike”

- Free, open source operating system
- Based on Linux (Ubuntu LTS) (64-bit)
- Release cycle in synchronization with Ubuntu
- Free and Open Source Software Advocacy
- 8 years
- 6 major releases, 3 base distributions
- 143 packages, >500 bioinformatics tools



<http://nebc.nerc.ac.uk/tools/bio-linux>

1.1 Community Outreach

- Bio-Linux USB Sticks
- Users/Developers Group Meetings (BOSC)
- Mailing lists (Developers, Users)
- HelpDesk for User Support: helpdesk@nebc.ac.uk
- Teaching: “Introduction to Bio-Linux”
- Code Catalogue
<http://nebc.nerc.ac.uk/tools/code-corner>

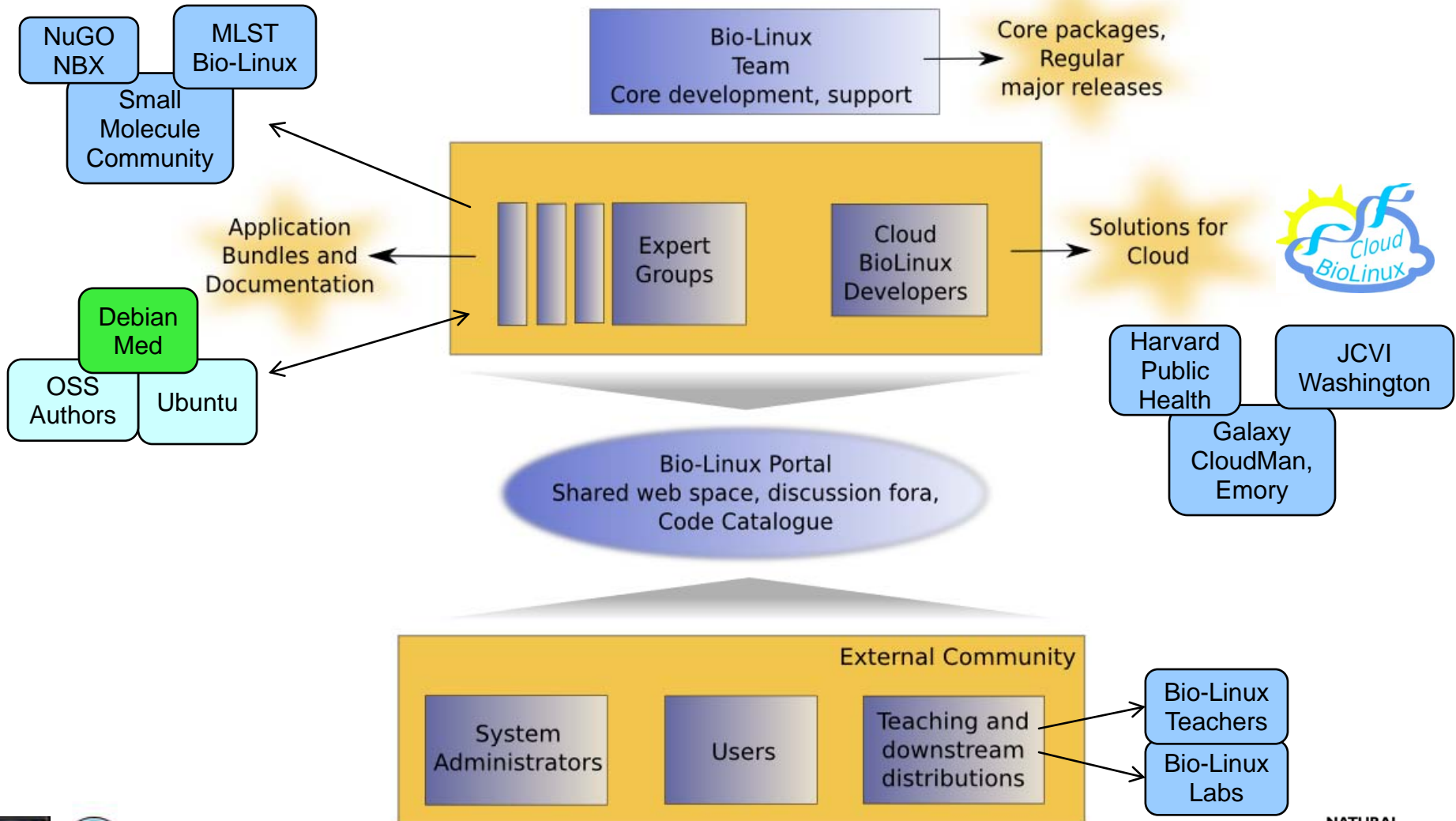
<http://nebc.nerc.ac.uk/tools/bio-linux>

1.2 Bio-Linux Usage Figures

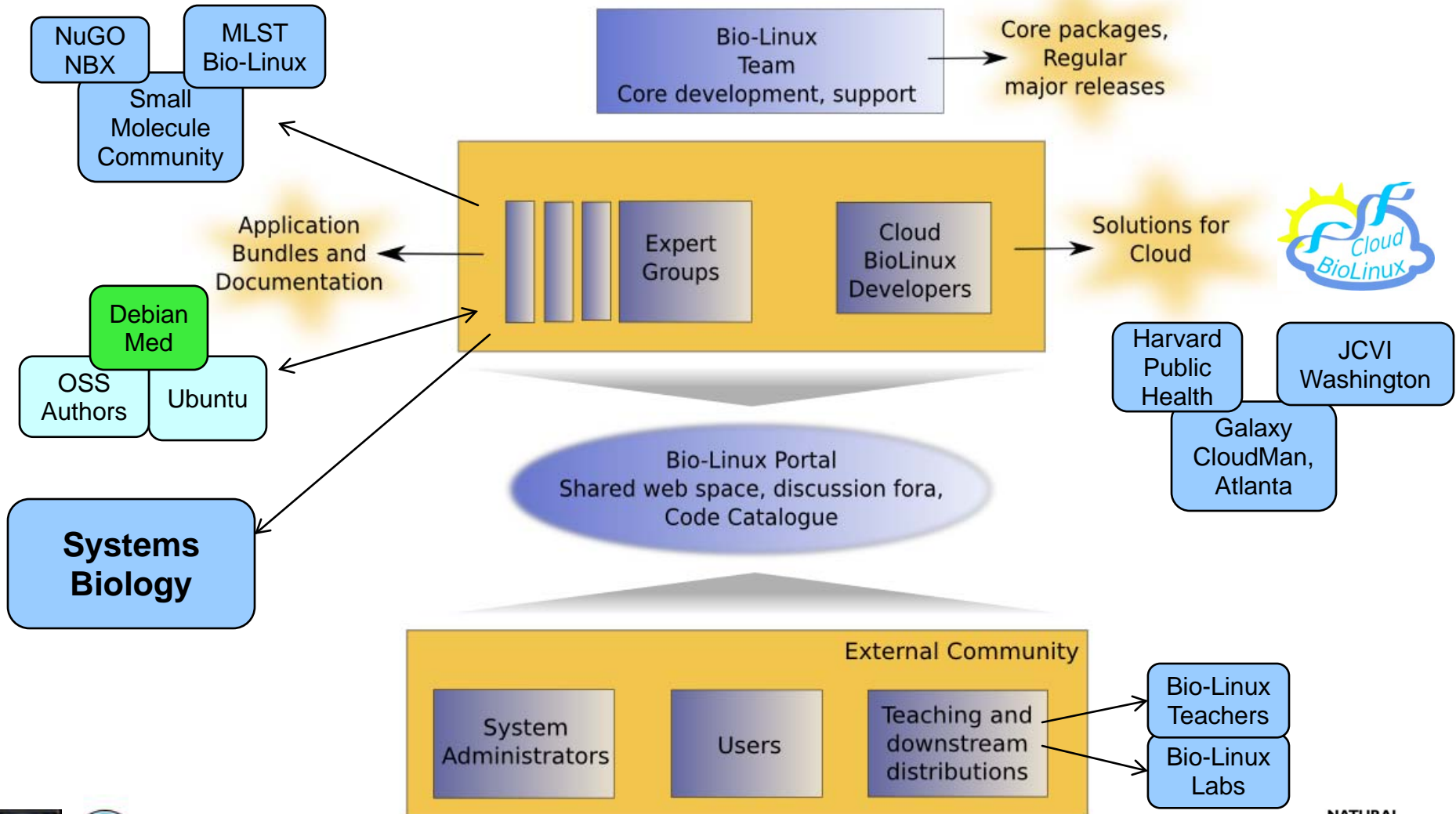
- >2500 registered ISO downloads
- 150 people on discussion list
- >5000 distinct IP hits on package repository (last month)
- 1200 page views (last month)

<http://nebc.nerc.ac.uk/tools/bio-linux>

1.3 The Bio-Linux Organogram



1.3 The Bio-Linux Organogram



2.1 Modelling Approaches: Top-Down

Top-Down Modelling (Mathematical modelling)

- ✚ Based on ordinary or partial differential equations
- ✚ Population of “identical” individuals
- ✚ Underlying behavioural rules are treated as a ‘black box’

- ✚ Essential in formulation of general theories
- ✚ Biological systems represent a challenge for mathematical modellers;
 - inherent complexity,
 - non-linear relationships among individual components

2.2 Modelling Approaches: Bottom-Up

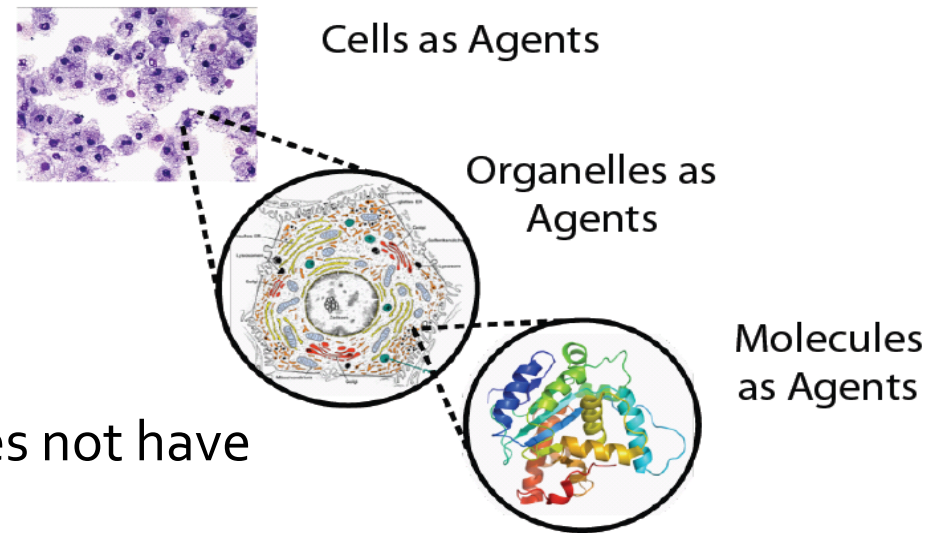
Bottom-Up Modelling (Agent-Based Modelling)

- ✚ Models each individual aiming to study:
 - mechanisms for underlying behaviour
 - interactions between individuals/environment
- ✚ Treats individuals as unique and discrete entities with properties that can change during their lives
- ✚ Once rules are specified, population and community level consequences emerge naturally

2.3 Why ABM

- In heterogeneous populations ability to focus on individuals – in all their variation – and to explore what emerges from their interactions

Agents at all Scales of Biology

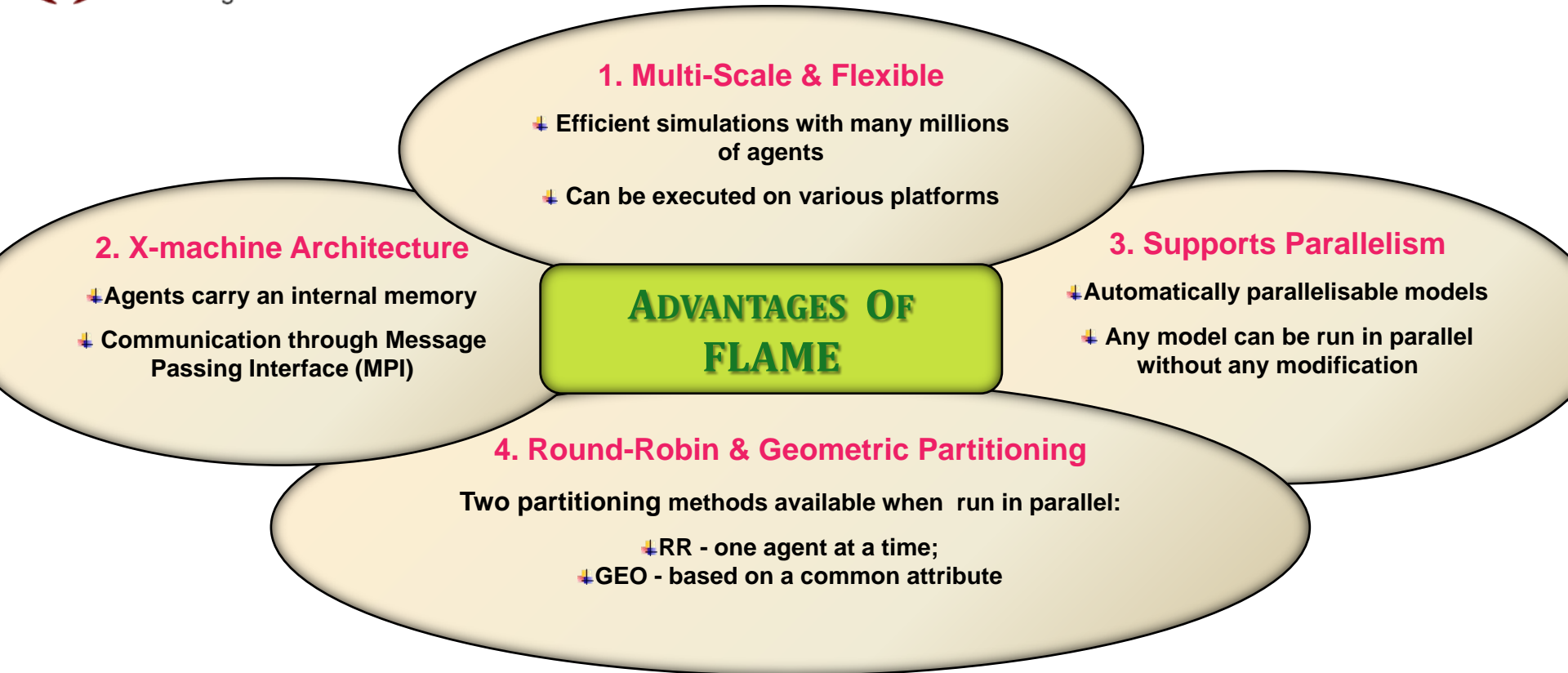


- Agent-based chemical model does not have same restrictions as ODE models; any number and distribution of molecules can be modelled, spatial concerns can easily be accounted
- Clearer picture of what is actually occurring in the cell

2.4 ABM Framework: FLAME

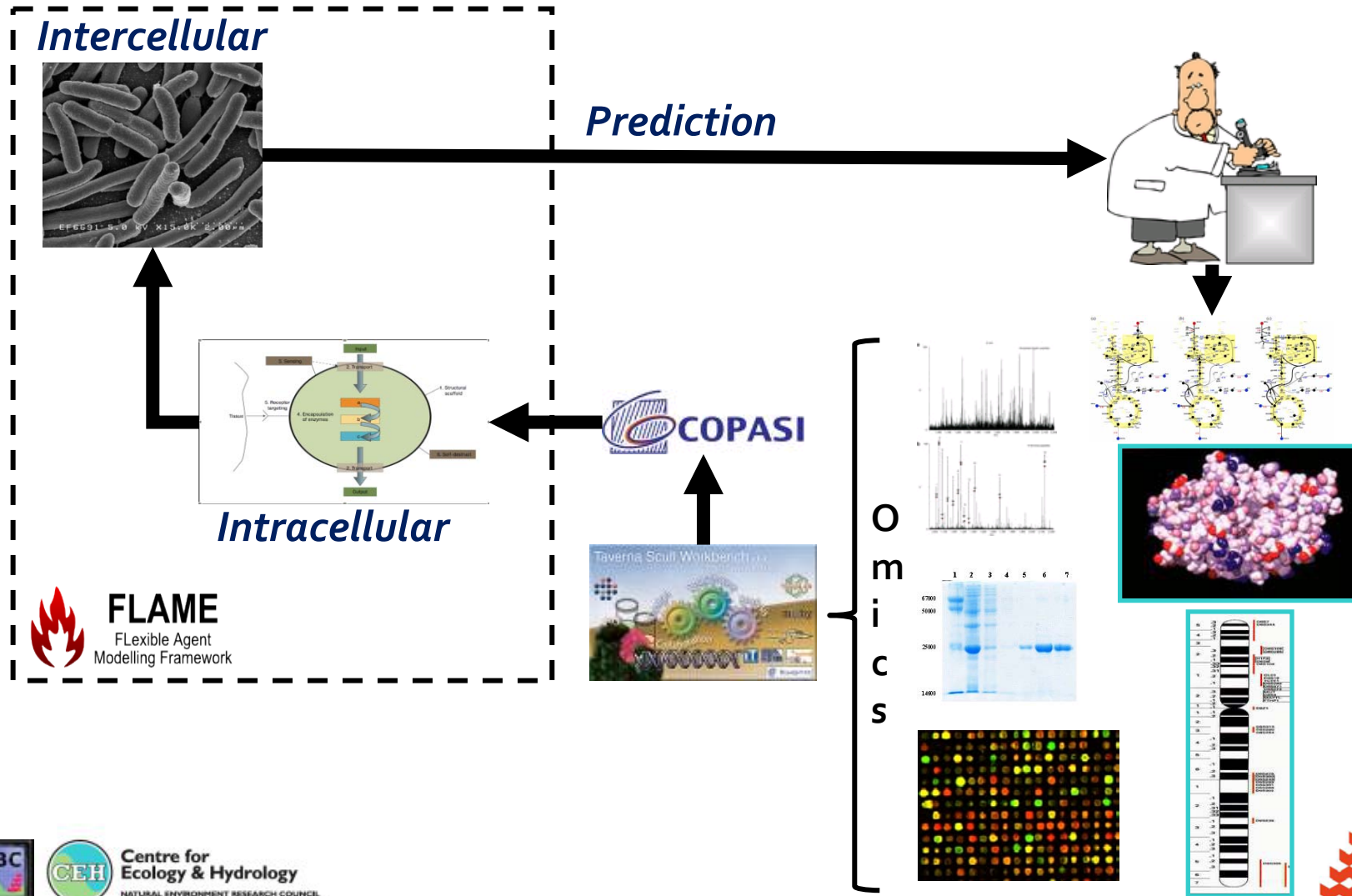


www.flame.ac.uk



2.5 Hybrid Modelling: SysMO (SUMO Consortium)

Modelling Regulation of Electron Transport Chain in *E. coli*



COPASI for SBML Generation

A

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<sbml>
  <model>
    <listOfCompartments>
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        <listOfProducts>
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</sbml>
```

Qualitative SBML model

Parameterisation
workflow



B

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      ...
    </listOfReactions>
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</sbml>
```

Parameterised SBML model

3.1 Standards: Technical Challenges

- **Support for hierarchical models (Lucian Smith)**
- **Support for dynamic structures (Chris Myers)**
- **What is appropriate for ABMS?**
- **Is an SBML extension for ABMs possible?**

Collaboration

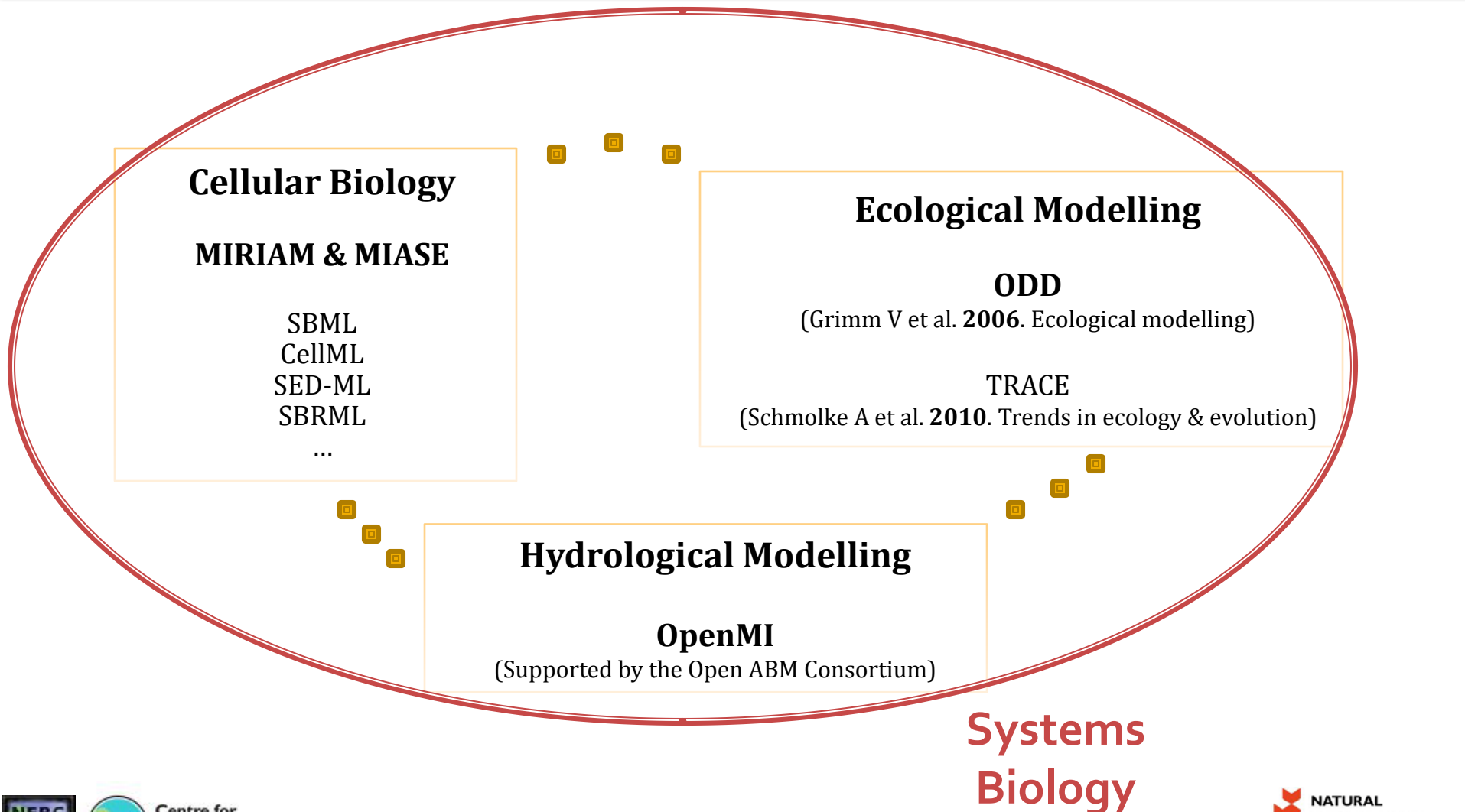
Biologists



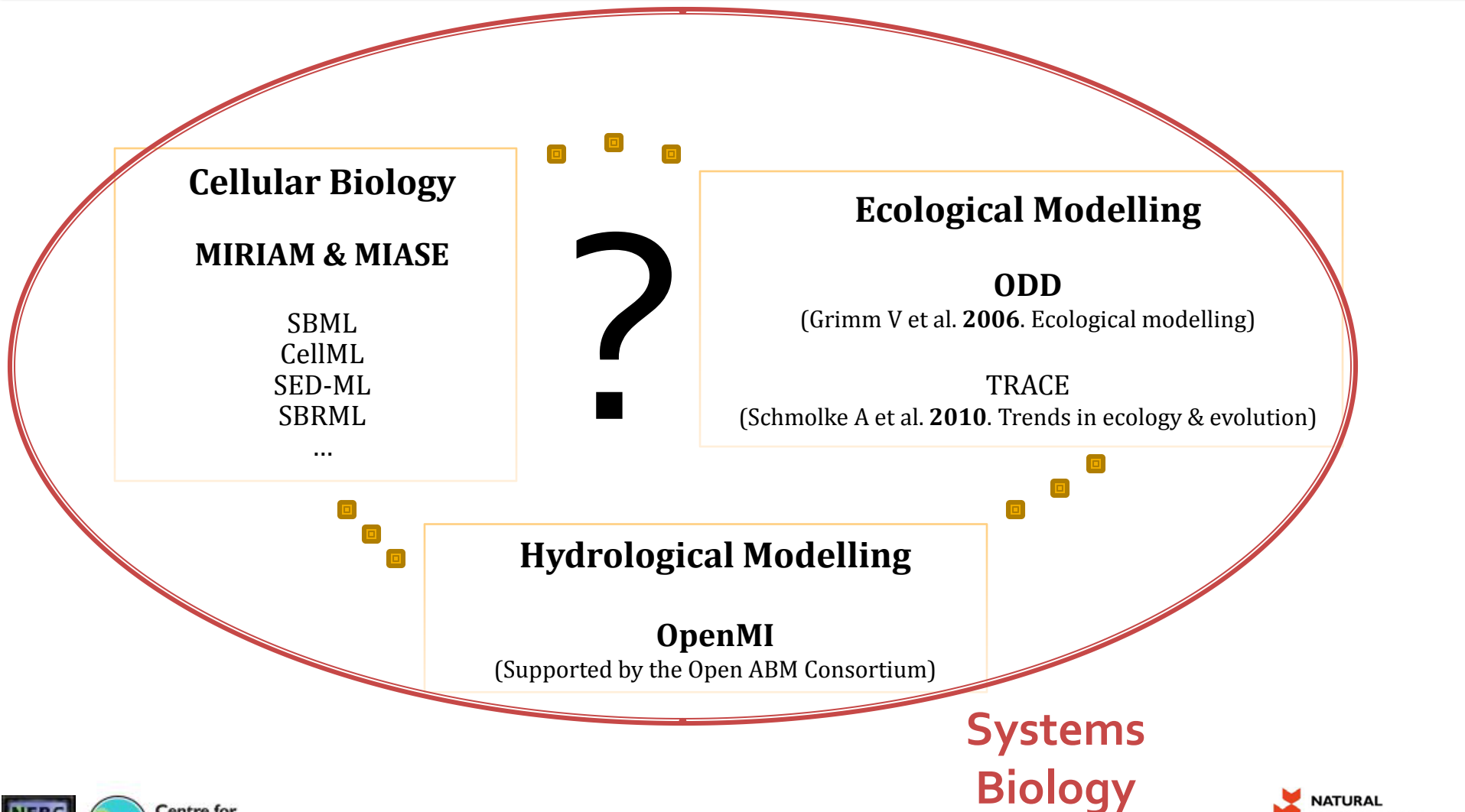
Modellers

Different Domains

3.2 Standards: Sociological Challenges



3.2 Standards: Sociological Challenges



Conclusive Remarks

- ✚ Is the COMBINE Community willing to help us form a “Systems Biology” software bundle on Bio-Linux?
- ✚ How can we integrate Agent-Based Modelling into the wider community?
- ✚ How do we think about describing **“A Systems Biology Model”**?



Acknowledgements



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SysMO Consortium

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Professor Carol Coble

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