SPiNMe: An Environment for the Rapid Prototyping of New Numerical Methods

Antônio Tadeu A. Gomes
Diego Paredes
Frederico Teixeira
Frédéric Valentin

atagomes@lncc.br

http://www.lncc.br/sinapad/SPiNMe
http://www.facebook.com/sinapad

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SINAPAD

Numerical Methods

$$-\epsilon\Delta u + \alpha \cdot \nabla u + \sigma u = f$$

Approximate solution

$$\mathbf{A}\mathbf{u} = \mathbf{f}$$

- Accuracy
- Flexibility
- Performance
- Mathematical theory

Finite Element Methods

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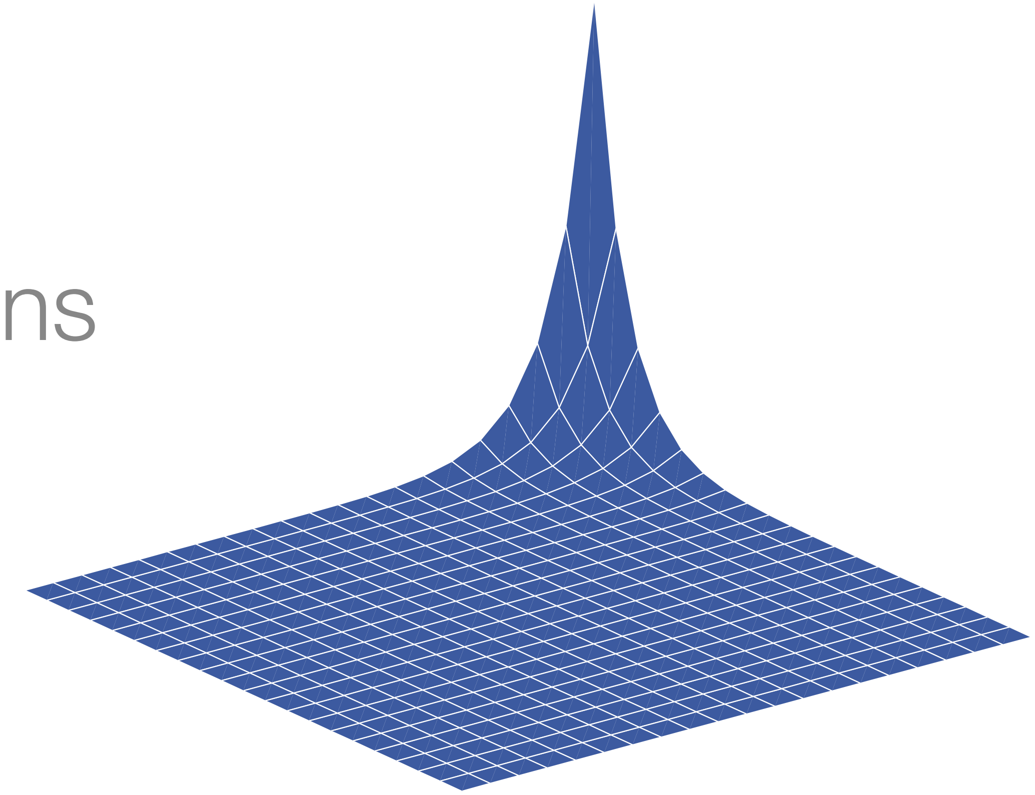
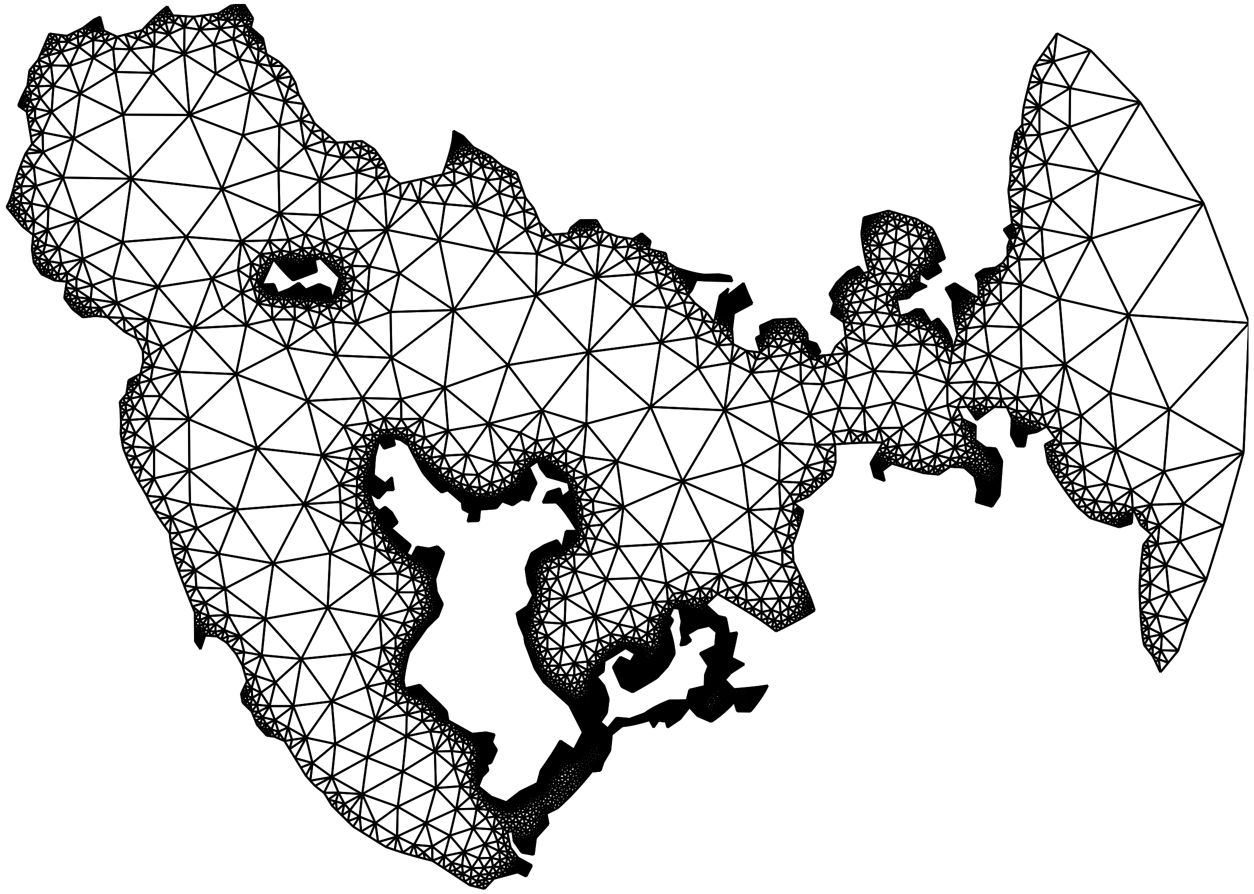
- Geometric flexibility

- Amenability to **method** adaptations





New methods...

Voilà!!!
My new method!!!

$$a(u,v) + \sum_K \frac{1}{2} \int_{\partial K} \gamma h_{\partial K} [\nabla u \cdot n][\nabla v \cdot n] \; ds = (f,v)$$

- Do I need **brand new code**?

Primary study on FEM implementations

- SAAM* method applied to different libs/packages
  - deal.II
  - FreeFEM++
  - GetFEM
  - Hermes
  - OOFEM
  - NeoPZ

- Overall perception: **code** adaptability is "in the eye of the beholder"
  - Elements
  - Basis functions
  - Variational formulations

  ...

* Kazman, R.; Abowd, G.; Bass, L.; Clements, P.; , "Scenario-based analysis of software architecture," Software, IEEE, vol.13, no.6, pp.47-55, Nov 1996, doi: 10.1109/52.542294
URL: http://ieeexplore.ieee.org/stamp/stamp.jsp?tp=&arnumber=542294&isnumber=11767

New methods... as compared with "not-so-new" methods

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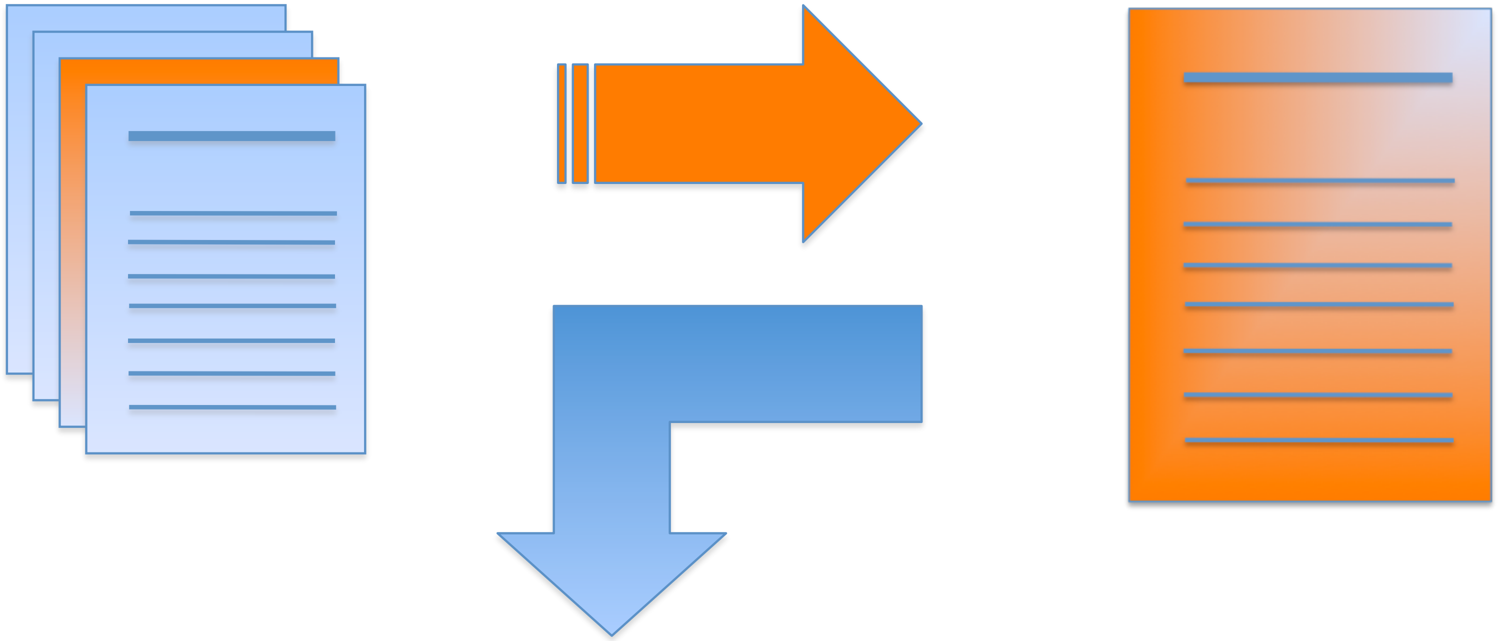
Digital libraries of "non-executable" papers



Gotcha!!!

$$a(u,v) + \sum_K \frac{1}{2} \int_{\partial K} \gamma h_{\partial K} [\nabla u \cdot n][\nabla v \cdot n] \; ds = (f,v)$$

- Do I need **brand new code**?

- How can I **compare** against other method implementations?

Comparability...

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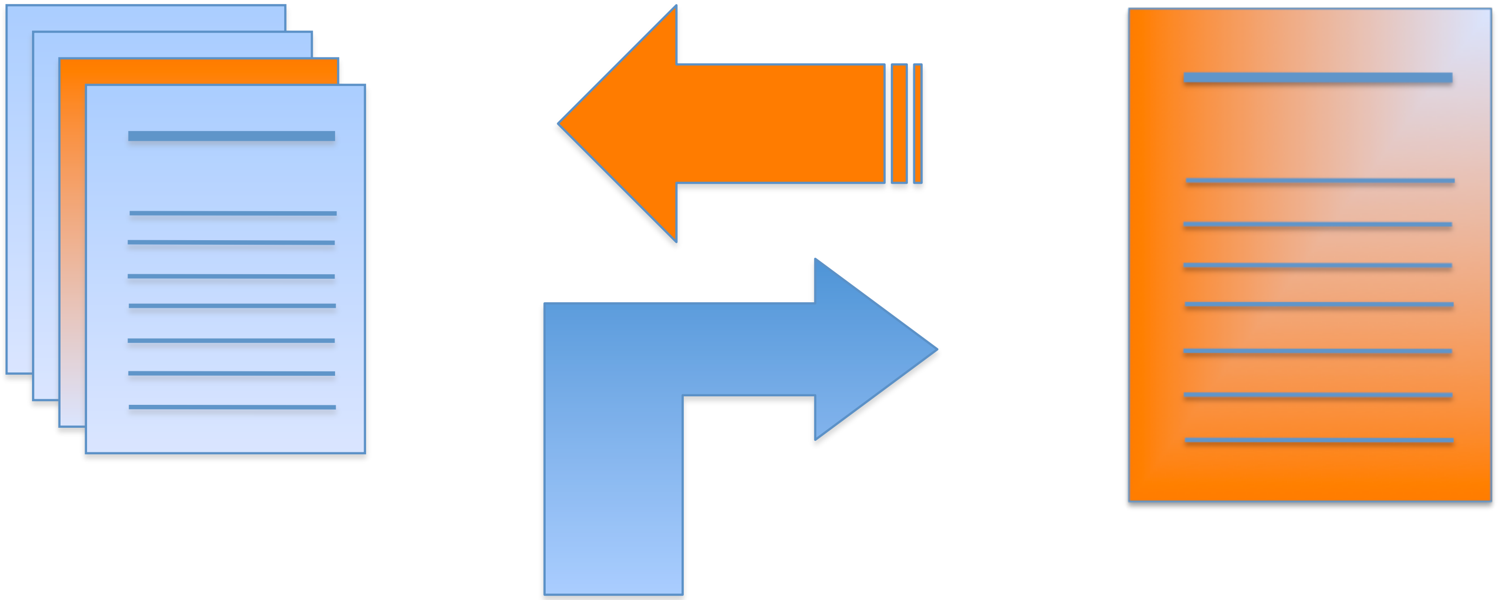
- A single/small set of numerical library implementations should be provided to the researcher for the implementation of his/her numerical method
    - PaaS approach

New methods... available/ reachable by the community



Digital libraries of "**non-executable**" papers

Accepted!!!

$$a(u,v) + \sum_{K} \frac{1}{2} \int_{\partial K} \gamma h_{\partial K} [\nabla u \cdot n][\nabla v \cdot n]\ ds = (f,v)$$

- Do I need **brand new code**?
- How can I **compare** against other method implementations?
- Will my implementation be **useful/ usable in the future**?

Reproducibility...

- The provided numerical libraries should be parametrized either via input data or via "plug-in" code representing the particularities of a specific numerical method

Playing with new methods...

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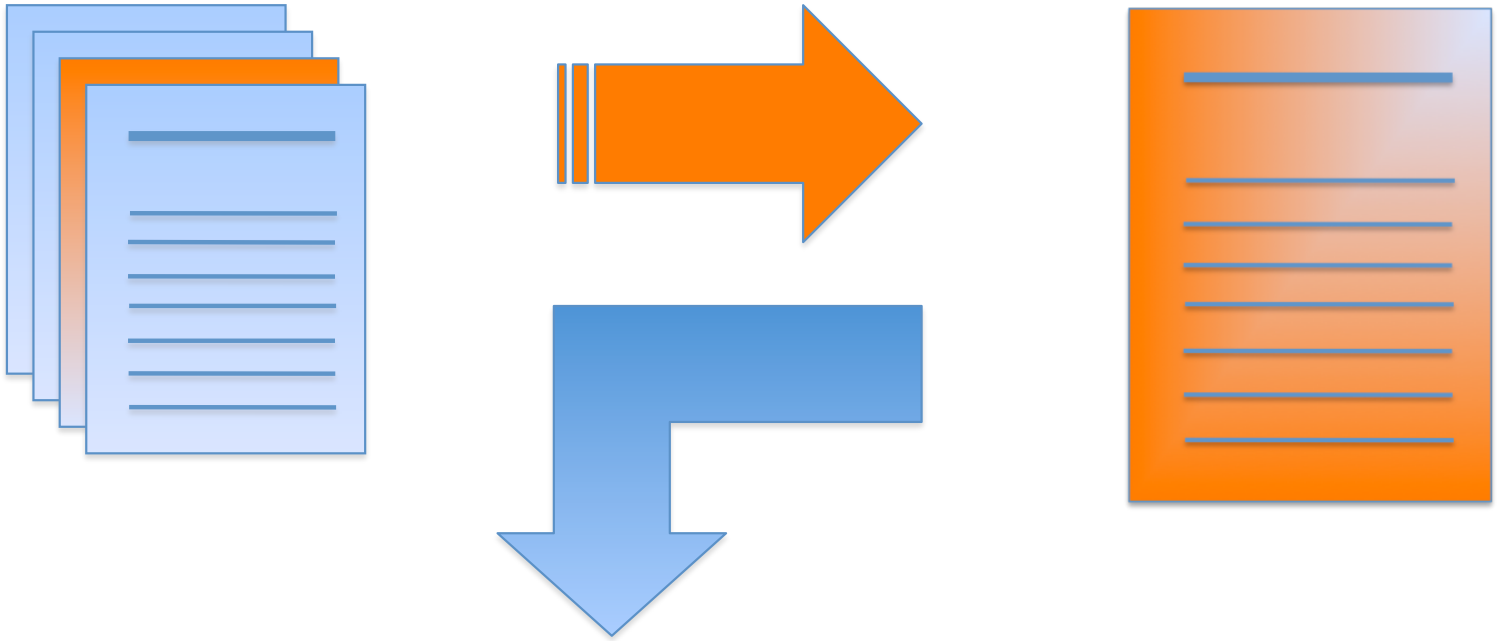
Digital libraries of "**executable**" papers



How about this???

$$a(u,v) + \sum_K \frac{1}{\underset{4}{\cancel{2}}} \int_{\partial K} \gamma h_{\partial K} [\nabla u \cdot n][\nabla v \cdot n] \; ds = (f,v)$$

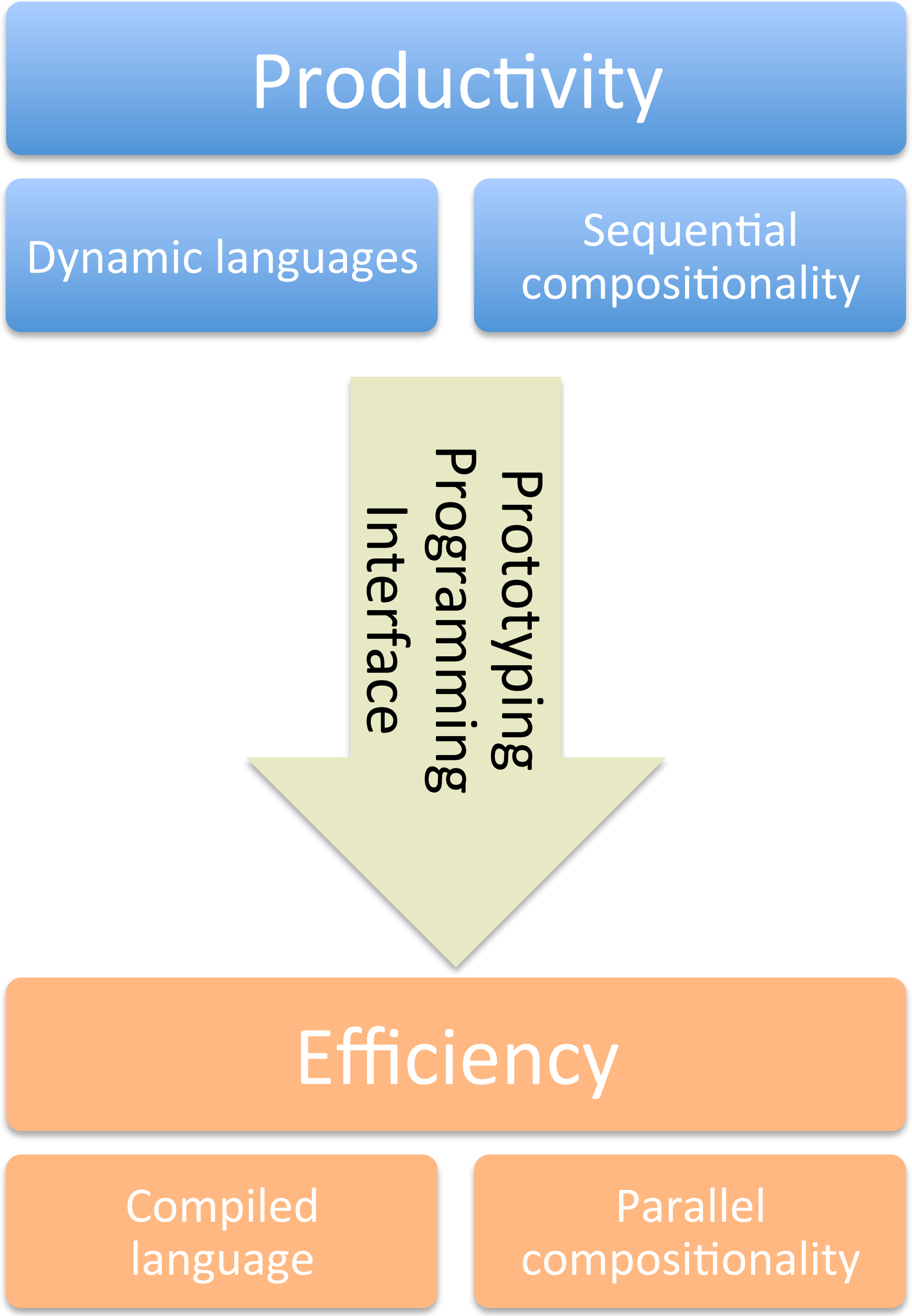
- Do I need **brand new code**?
- How can I **compare** against other method implementations?
- Will my implementation be **useful/ usable in the future**?
- Can I **(re)deploy at runtime**? (and **in real time**?)

Productivity...

- Hmmmm, one “Achilles heel” (or “Holy grail”?) in software engineering...

sci-tech software: technical complexity

- Long time-to-market
- "Crosscutting error" proneness
    - Software architecture!!
- Mitigation strategy
    - Stratification of productivity and efficiency
        - PPI is key (more on this in the end...)
    - Productivity through rapid prototyping
        - Lua
    - Efficiency through compiled kernel
        - NeoPZ


Productivity
Dynamic languages
Sequential compositionality
Prototyping Programming Interface
Efficiency
Compiled language
Parallel compositionality

Why Lua?

- Simple syntax
- Extensible semantics
- Portability (amenable to JiT compilation)
- Low memory footprint

[and I know it well... ;-)]

From the authors of Lua... (http://www.lua.org)

“Lua is a powerful, fast, lightweight, embeddable scripting language. Lua combines simple procedural syntax with powerful data description constructs based on associative arrays and extensible semantics. Lua is dynamically typed, runs by interpreting bytecode for a register-based virtual machine, and has automatic memory management with incremental garbage collection, making it ideal for configuration, scripting, and rapid prototyping.”

Why NeoPZ?

LABMEC

- Good architectural intention and design
- C++ (embedding easier)

UNICAMP

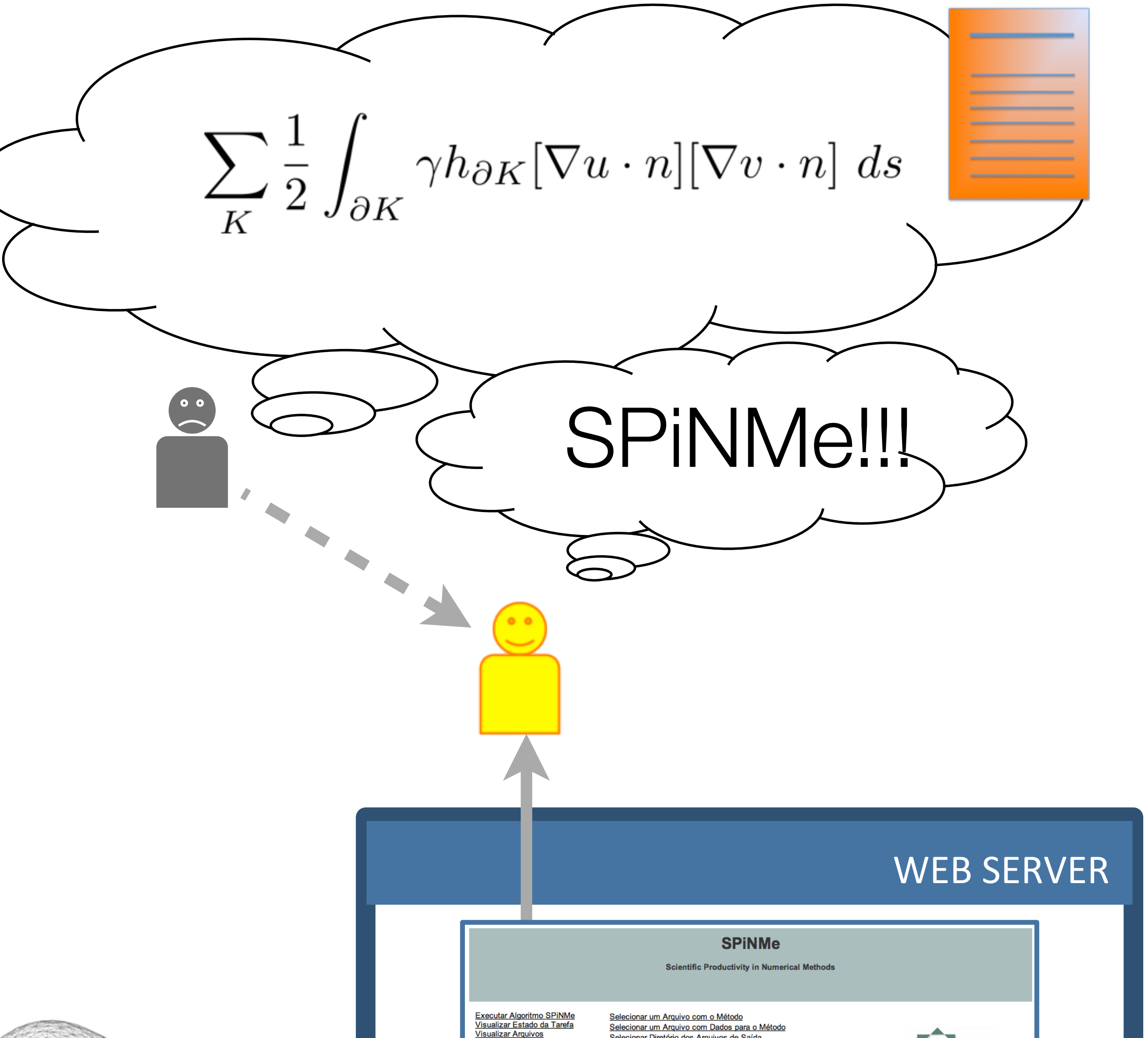
From the authors of NeoPZ: (http://code.google.com/p/neopz/)

“NeoPZ is an object oriented programming environment which implements hp adaptive finite element algorithms. The PZ classes can be used standalone but can also be linked with blas, boost, pthread, log4cxx and metis. The advanced finite element technologies implemented are: h and hp adaptivity for one, two and three dimensional meshes; the variational formulation of the conservation law is separated from the generation of the approximation space. Therefore NeoPZ can be used for virtually any system of differential equation. Various storage patterns for the global stiffness matrix : full, banded, skyline, sparse, frontal. Iterative solvers with configurable preconditioners. Post processing interface to opendx and vtk.”

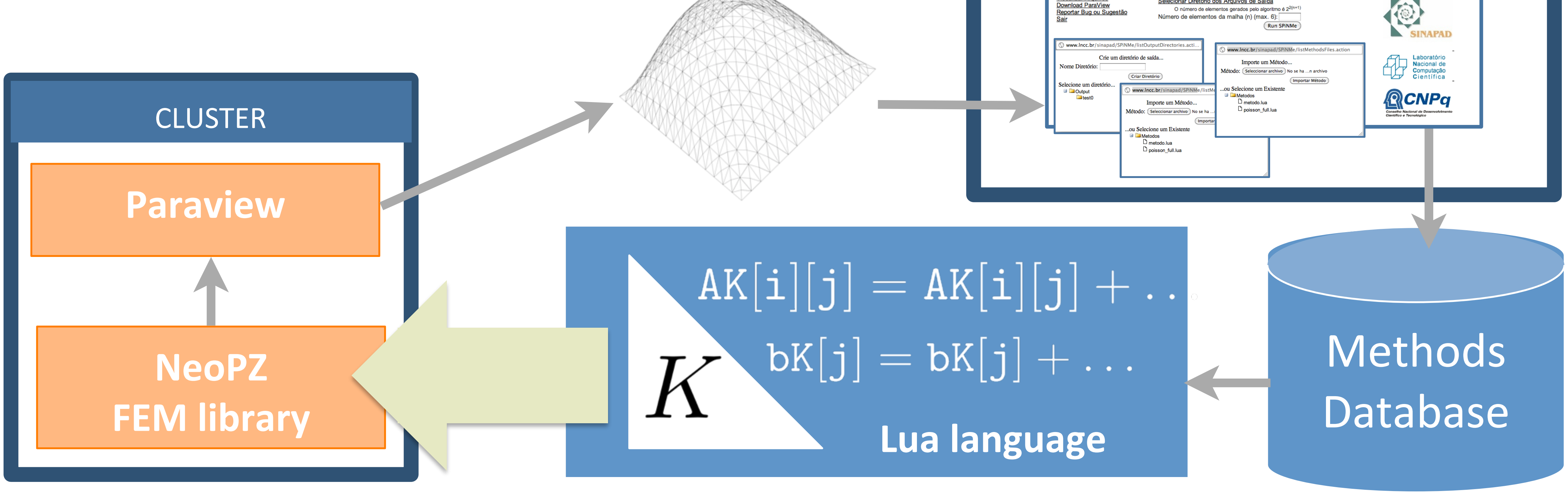
[...and we know well who knows it well ;-)]

SPiNMe

- Rapid prototyping of FE methods
    - Local programming
    - Good performance
- Perpetuation/reproduction of methods
    - Concept of "***executable paper***"



$$\sum_K \frac{1}{2}\int_{\partial K} \gamma h_{\partial K}[\nabla u \cdot n][\nabla v \cdot n]\; ds$$



SPiNMe

Scientific Productivity in Numerical Methods

Executar Algoritmo SPiNMe
Visualizar Estado da Tarefa
Visualizar Arquivos
Download ParaView
Reportar Bug ou Sugestão
Sair

Selecionar um Arquivo com o Método
Selecionar um Arquivo com Dados para o Método
Selecionar Diretório dos Arquivos de Saída

O número de elementos gerados pelo algoritmo é $2^{2(n+1)}$

Número de elementos da malha (n) (max. 6):

Run SPiNMe

www.lncc.br/sinapad/SPiNMe/listOutputDirectories.acti...

Crie um diretório de saída...

Nome Diretório:

Criar Diretório

Selecione um diretório...
- Output
    - test0

www.lncc.br/sinapad/SPiNMe/listMe

Importe um Método...

Método: Seleccionar archivo No se ha ...

Importar

...ou Selecione um Existente
- Metodos
    - metodo.lua
    - poisson_full.lua

www.lncc.br/sinapad/SPiNMe/listMethodsFiles.action

Importe um Método...

Método: Seleccionar archivo No se ha ...n archivo

Importar Método

...ou Selecione um Existente
- Metodos
    - metodo.lua
    - poisson_full.lua

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CLUSTER
Paraview
NeoPZ
FEM library
K
Lua language
Methods
Database

```
AK[i][j] = AK[i][j] + ...
bK[j] = bK[j] + ...
```

Code snippets (I)

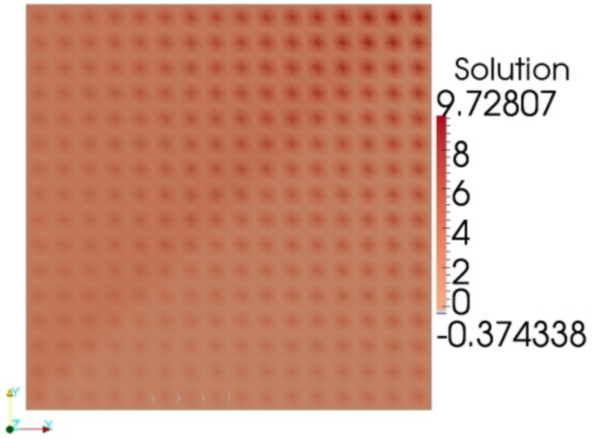
$$-\epsilon\Delta u + \alpha \cdot \nabla u + \sigma u = f$$

$$\Downarrow$$

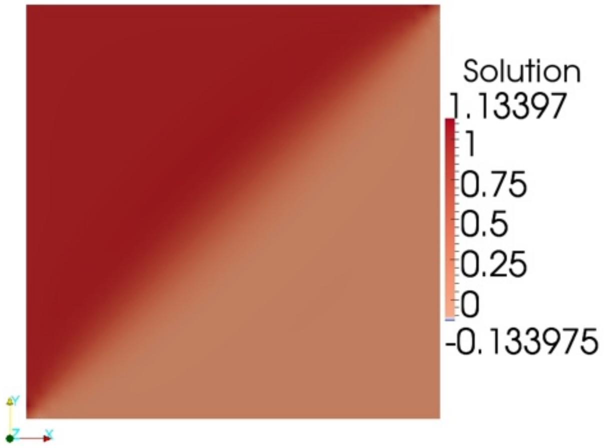
$$B(u_h, v_h) + U(u_h, v_h) = (f, v_h) + F(v_h)$$

```
Dimension = 2,

FreeNodes = { -- "[1]": id of elements in the mesh
  [1] = { Reaction = { Sigma = 0.01, },
        Advection = { Alpha = { 0.5 , 0.5 }, },
        Diffusion = { Epsilon = {  { 0.0001, 0.0 }, { 0.0, 0.0001 }, }, },
        SourceSink = { F = 1.0, },
        stabilization_term = { }, }, -- not provided in NeoPZ...
},

ConstrainedNodes = { -- "[14]","[15]": ids of elements in the mesh
  [14] = { PhyEntity = 1, Dirichlet = { G = 1.0, }, },
  [15] = { PhyEntity = 1, Dirichlet = { G = 0.0, }, },
},

FreeNodes[1].stabilization_term = {
  Nu = FreeNodes[1].Diffusion.Epsilon[1][1],
  Sigma = FreeNodes[1].Reaction.Sigma,
  A = FreeNodes[1].Advection.Alpha,
  f = FreeNodes[1].SourceSink.F,
  N = 8192 -- number of elements, mesh dependent!!!!
}
```

```
local function tau_K() ... -- aux function omitted for brevity

function stabilization_term.asmFreeNodes(data, weight, ek, ef)
 local x, phi, dphi = data:getX(), data:getPhi(), data:getDPhix()
 local r = phi.rows

 for i=0,r-1 do
  ef[i][0] = ef[i][0] + weight * f * phi[i][0] -
    N * weight * f * tau_K(x[0],x[1]) *
    (Sigma * phi[i][0] - A[0] * dphi[0][i] - A[1] * dphi[1][i])
  for j=0,r-1 do
   ek[i][j] = ek[i][j] - N * weight *
     ( Sigma * Sigma * phi[j][0] * phi[i][0] * tau_K(x[0],x[1]) +
       Sigma * (A[0] * dphi[0][j] + A[1] * dphi[1][j] ) * tau_K(x[0],x[1]) * phi[i][0] -
       Sigma * phi[j][0] * tau_K(x[0],x[1]) * (A[0] * dphi[0][i] + A[1] * dphi[1][i]) -
       (A[0] * dphi[0][j] + A[1] * dphi[1][j]) *
       tau_K(x[0],x[1]) * (A[0] * dphi[0][i] + A[1] * dphi[1][i]) )
  end
 end
end
```



Without stabilization term



With stabilization term

Code snippets (II)

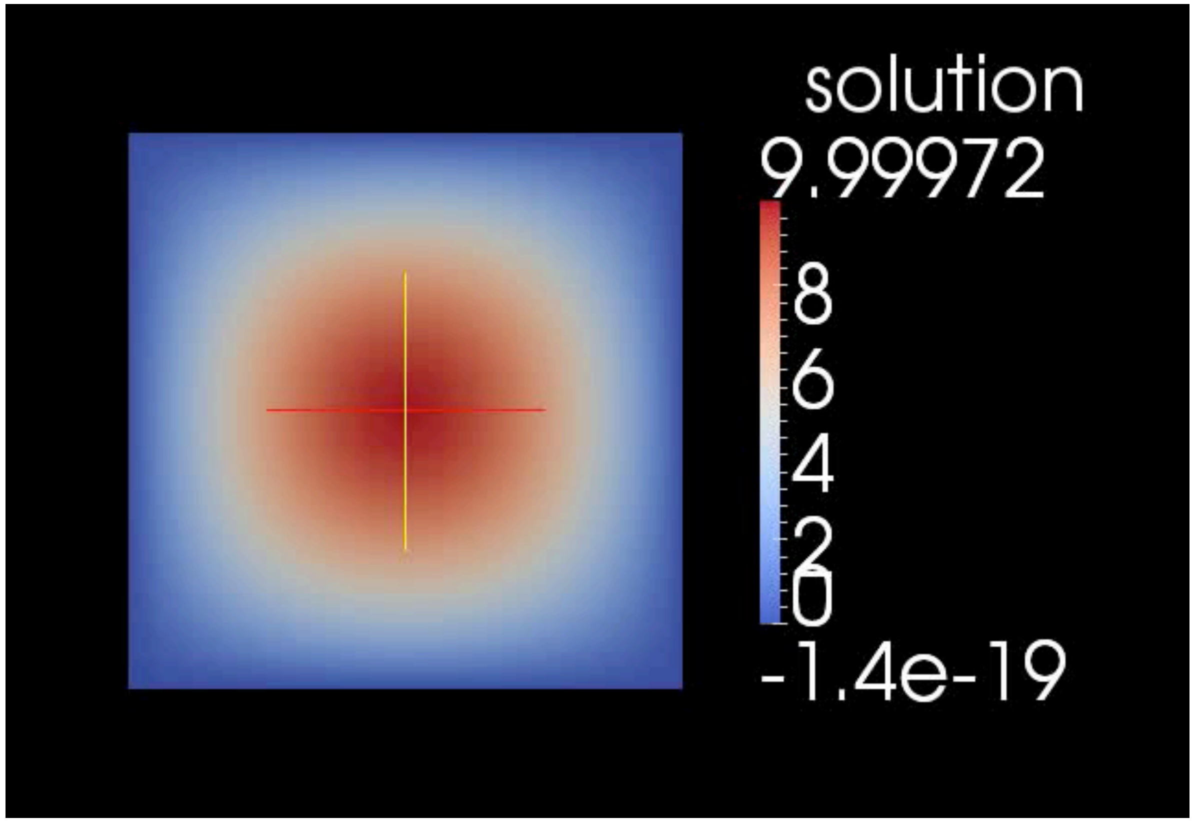
$$-\epsilon\Delta u = f$$

↓

$$B(u_h,v_h) = (f,v_h)$$

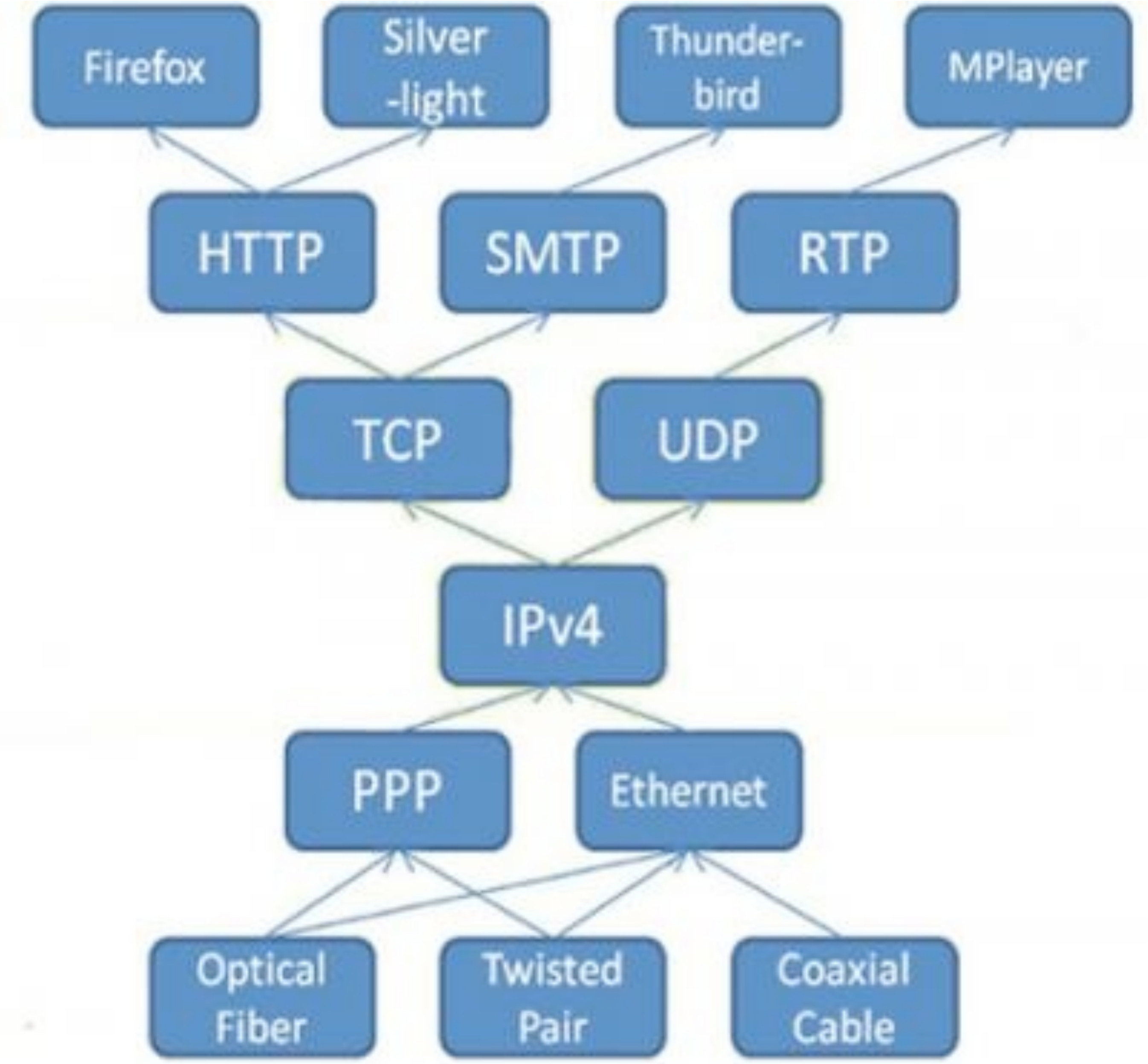
```
ElementType = Quadrilateral
Precision = 1
InterpolationOrder = 3
StructuralMatrix = BAND
Solver = LU
TimeStep = 1/100
TimeIterations = 2000
ThetaMethod = 0.5
-- ExactSolution = function(x,y,z,t) return 10*math.exp(-t)*math.sin(math.pi*x)*math.sin(math.pi*y) end
InitialCondition = function(x,y,z,t) return 10*math.sin(math.pi*x)*math.sin(math.pi*y) end
```

```
Dimension = 2,

FreeNodes = {
  [1] = { TransientFirst = { Coeff = 1.0 },
          Diffusion = { Epsilon = { {1.0, 0.0}, {0.0, 1.0} } },
          SourceSink = { F = function(x,y,z,t) return 0.0 end }, },
  },

ConstrainedNodes = {
  [1] = { PhyEntity = 1,
          Dirichlet = { G = function(x,y,z,t) return 0.0 end, }, },
},
```



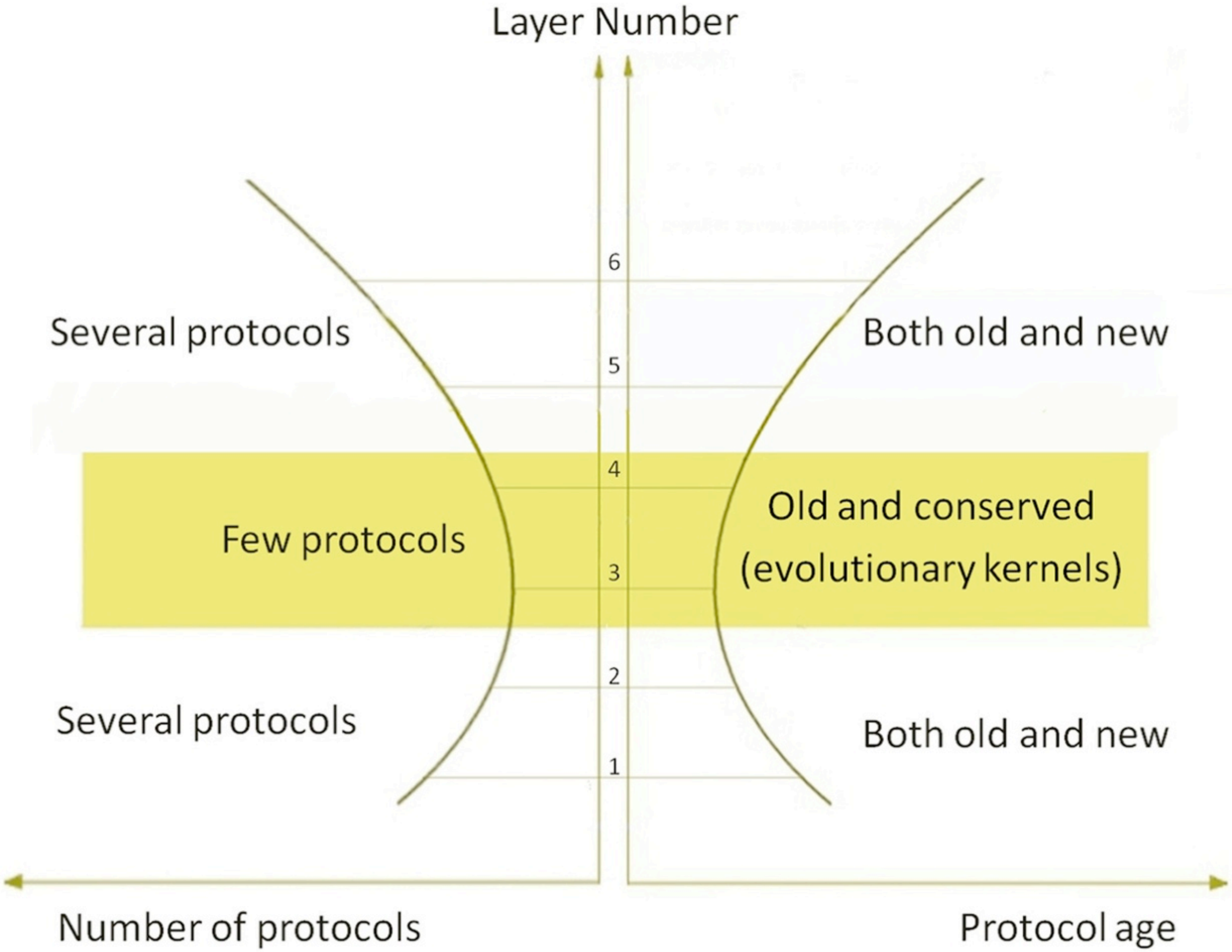
Difficulties

- Design/evolution of PPI
  - Resemblance with Internet's hourglass model



Difficulties

- Design/evolution of PPI
    - Resemblance with Internet’s hourglass model
- Is ossification a problem?



Ongoing and future work

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- Stationary (done)
- Scalar (done)
- Transient (done)
- Vectorial (done)
- Meshes: gmesh, tetgen (done)

- Nonlinear PDEs
- MPI/GPU awareness
- Symbolic coding
- JiT compilation of Lua code
- Pause/redeploy/resume
- Link to scientific hypothesis database

Questions?

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