Composite Algorithm to compute Three-term Recurrence Coefficients

Zexin Liu

Department of Mathematics
University of Utah

May 9, 2019

Outline

- Evaluations of orthogonal polynomials
- Three-term recurrence coefficients
- Algorithms to compute coefficients
- Numerical experiments

Evaluations of orthogonal polynomials

Why are OPs so important?:

- numerical integration using quadrature rules and approximation theory.
- polynomials expansion, widely used in solving PDEs with various methods, e.x. Jacobi Galerkin Method, ENO and WENO.
  - Galerkin: need to define an approximation space.
  - ENO and WENO: need to use numerical flux with polynomials reconstructions to evaluate cells boundaries
- foundational tool in gPC

How to evaluate OPs?

- an intuitive way: Gram-Schmidt process
- other fancy techniques

Evaluate OPs with G-S

Orthogonal polynomials can be obtained by applying the *Gram-Schmidt orthogonalization process* to the basis $1, x, x^2, \ldots$:

$$p_0(x) = 1,$$

$$p_1(x) = x - \frac{\langle x, p_0\rangle}{\langle p_0, p_0\rangle} p_0(x),$$

$$p_2(x) = x^2 - \frac{\langle x^2, p_0\rangle}{\langle p_0, p_0\rangle} p_0(x) - \frac{\langle x^2, p_1\rangle}{\langle p_1, p_1\rangle} p_1(x),$$

....

$$p_n(x) = x^n - \frac{\langle x^n, p_0\rangle}{\langle p_0, p_0\rangle} p_0(x) - \cdots - \frac{\langle x^n, p_{n-1}\rangle}{\langle p_{n-1}, p_{n-1}\rangle} p_{n-1}(x),$$

....

Then $p_0, p_1, p_2, \ldots$ are orthogonal polynomials.

n	$P_n(x)$
0	1
1	x
2	$\frac{1}{2}\left(3x^2-1\right)$
3	$\frac{1}{2}\left(5x^3-3x\right)$
4	$\frac{1}{8}\left(35x^4-30x^2+3\right)$
5	$\frac{1}{8}\left(63x^5-70x^3+15x\right)$
6	$\frac{1}{16}\left(231x^6-315x^4+105x^2-5\right)$
7	$\frac{1}{16}\left(429x^7-693x^5+315x^3-35x\right)$
8	$\frac{1}{128}\left(6435x^8-12012x^6+6930x^4-1260x^2+35\right)$
9	$\frac{1}{128}\left(12155x^9-25740x^7+18018x^5-4620x^3+315x\right)$
10	$\frac{1}{256}\left(46189x^{10}-109395x^8+90090x^6-30030x^4+3465x^2-63\right)$

The operations for orthogonal matrices are terribly UNSTABLE due to the round-off error!

TTR and OPs

Assume $p_{-1}(x) = 0$, $p_0(x) = \frac{1}{b_0}$ and define $b_0^2 = \int w(x)dx$

$$(TTR) \quad xp_n(x) = b_n p_{n-1}(x) + a_{n+1} p_n(x) + b_{n+1} p_{n+1}(x), n = 0, 1, \ldots$$

Proof.

$xp_n(x) = \sum_{j=0}^{n+1} d_{nj} p_j(x)$ since $xp_j(x)$ is a poly of degree $j+1$, where

$$\begin{aligned} d_{nj} &= \langle xp_n, p_j \rangle_w \\ &= \langle p_n, xp_j \rangle_w \\ &= \begin{cases} 0 & \text{if } j+1 \leq n-1 \\ d_{nj} & \text{if } n-1 \leq j \leq n+1 \end{cases} \end{aligned}$$

So $xp_n(x) = d_{n,n+1} p_{n+1}(x) + d_{n,n} p_n(x) + d_{n,n-1} p_{n-1}(x)$ □

Manipulations of OPs $\iff$ Manipulations of TTR coefficients (backward stable)

Ways to compute the recurrence coeffcients

- Derive exact formulas for coefficients
  - Rodrigues' formula (for classical OPs: Jacobi, Laguerre, Hermite)
  - discrete Painlevé I equation and Freud's conjecture (for Freud's weight)
  - recurrence formula (for certain piecewise smooth weight)

$w(t)$	Support	Name	α_k	β_0	$\beta_k,\ k \geq 1$
1	$[-1,1]$	Legendre	0	2	$1/(4-k^{-2})$
1	$[0,1]$	Shifted Legendre	$\frac{1}{2}$	1	$1/(4(4-k^{-2}))$
$(1-t^2)^{-1/2}$	$[-1,1]$	Chebyshev #1	0	π	$\frac{1}{2}\ (k=1),\ \frac{1}{4}\ (k>1)$
$(1-t^2)^{1/2}$	$[-1,1]$	Chebyshev #2	0	$\frac{1}{2}\pi$	$\frac{1}{4}$
$(1-t)^{-1/2}(1+t)^{1/2}$	$[-1,1]$	Chebyshev #3	$\frac{1}{2}\ (k=0)$ $0\ (k>0)$	π	$\frac{1}{4}$
$(1-t)^{1/2}(1+t)^{-1/2}$	$[-1,1]$	Chebyshev #4	$-\frac{1}{2}\ (k=0)$ $0\ (k>0)$	π	$\frac{1}{4}$
$(1-t^2)^{\lambda-1/2},\ \lambda > -\frac{1}{2}$	$[-1,1]$	Gegenbauer	0	$\sqrt{\pi}\,\frac{\Gamma(\lambda+\frac{1}{2})}{\Gamma(\lambda+1)}$	$\frac{k(k+2\lambda-1)}{4(k+\lambda)(k+\lambda-1)}$
$(1-t)^{\alpha}(1+t)^{\beta}$ $\alpha > -1,\ \beta > -1$	$[-1,1]$	Jacobi	α_k^J	β_0^J	β_k^J
e^{-t}	$[0,\infty]$	Laguerre	$2k+1$	1	k^2
$t^{\alpha}\mathrm{e}^{-t},\ \alpha > -1$	$[0,\infty]$	Generalized Laguerre	$2k+\alpha+1$	$\Gamma(1+\alpha)$	$k(k+\alpha)$
e^{-t^2}	$[-\infty,\infty]$	Hermite	0	$\sqrt{\pi}$	$\frac{1}{2}k$
$\lvert t\rvert^{2\mu}\mathrm{e}^{-t^2},\ \mu > -\frac{1}{2}$	$[-\infty,\infty]$	Generalized Hermite	0	$\Gamma(\mu+\frac{1}{2})$	$\frac{1}{2}k\ (k\ \text{even})$ $\frac{1}{2}k+\mu\ (k\ \text{odd})$
$\frac{1}{2\pi}\mathrm{e}^{(2\phi-\pi)t}\lvert\Gamma(\lambda+it)\rvert^2$ $\lambda > 0,\ 0 < \phi < \pi$	$[-\infty,\infty]$	Meixner–Pollaczek	$-\frac{k+\lambda}{\tan\phi}$	$\frac{\Gamma(2\lambda)}{(2\sin\phi)^{2\lambda}}$	$\frac{k(k+2\lambda-1)}{4\sin^2\phi}$

- Classical moments method
- Modified Chebyshev moments method
- Composite algorithm

Rodrigues' formula

Let $w(x)$ be a weight function with support on $[a, b]$, $a, b \in \mathbb{R} \cup \infty$. Let $\{p_n(x)\}_{n \in \mathbb{N}_{\not\vdash}}$ be the associated orthonormal polynomial family.
Assume:

- $w'(x) = w(x)\frac{l(x)}{q(x)}$, $l(x) \in P_1$ and $q(x) \in P_2$.
- $\lim_{x \to a} w(x)q(x) = 0$
- $\lim_{x \to b} w(x)q(x) = 0$

Then: $p_n(x) = c_n \frac{1}{w(x)} \frac{d^n}{dx^n}[w(x)q(x)^n]$

Proof.

... □

Ex: Legendre polynomials, $w(x) = 1$ and $q(x) = 1 - x^2$.
$b_n^2 = \frac{\Gamma(2n-1)\Gamma(2n)}{2^{2n-1}\Gamma^4(n)} \frac{2^{2n+1}\Gamma^4(n+1)}{\Gamma(2n+1)\Gamma(2n+2)} = \frac{n^2}{4n^2-1}$
Pros: exact formula. Cons: only apply for "classical" OPs

Classical Moment Method

Define finite moments

$$\mu_r = \int x^r d\lambda(x) < \infty, r = 0, 1, 2, \ldots$$

Define Hankel determinants

$$\Delta_n = \begin{vmatrix} \mu_0 & \mu_1 & \cdots \mu_{n-1} \\ \mu_1 & \mu_2 & \cdots \mu_n \\ \vdots & \vdots & \\ \mu_{n-1} & \mu_n & \cdots \mu_{2n-2} \end{vmatrix}, n = 1, 2, \ldots, \qquad \Delta_0 = 1$$

and $\Delta_n^{'}$ with the penultimate column and last row removed.

Claim:

$$a_{n+1} = \frac{\Delta_{n+1}^{'}}{\Delta_{n+1}} - \frac{\Delta_n^{'}}{\Delta_n}, n = 0, 1, 2, \ldots; \qquad b_n^2 = \frac{\Delta_{n+1}\Delta_{n-1}}{\Delta_n^2}, n = 1, 2, 3, \ldots$$

Modified Chebyshev Method

Assumption:

- $\{\alpha_n, \beta_n\}$ under given measure $d\lambda(x)$ corresponding to monic orthogonal polynomials $\pi_l(x)$.
- $\{a_n, b_n\}$ under a certain type of measure(chosen) close to $d\lambda(x)$ corresponding to orthonormal polynomials $p_k(x)$.

Define "mixed moments" as

$$\sigma_{l,k} = \int \pi_l(x) p_k(x) d\lambda(x)$$

When $l = 0$,

$$\sigma_{0,k} = \int \pi_0(x) p_k(x) d\lambda(x) = \int f(x) d\tilde{\lambda}(x), \quad f(x) = p_k(x) \frac{d\lambda(x)}{d\tilde{\lambda}(x)}$$

Ex: $d\lambda(x) = (1 - \frac{1}{2}x^2)(1 - x^2)^{\frac{1}{2}}$, choose $d\tilde{\lambda}(x) = (1 - x^2)^{\frac{1}{2}}$

Modified Chebyshev Method

when $l = 1$,

$$\sigma_{1,k} = \int \pi_1(x) p_k(x) d\lambda(x)$$
$$= b_k \sigma_{0,k-1} + (a_{k+1} - \alpha_1)\sigma_{0,k} + b_{k+1}\sigma_{0,k+1}$$

If $k = 0$, $\sigma_{1,0} = b_0\sigma_{0,-1} + (a_1 - \alpha_1)\sigma_{0,0} + b_1\sigma_{0,1} = 0$.
Thus we can solve α_1 and thus evaluate $\pi_1(x)$ by TTR
when $l = 2$,

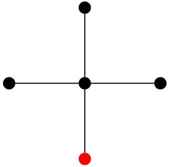
$$\sigma_{2,k} = \int \pi_2(x) p_k(x) d\lambda(x)$$
$$= b_k \sigma_{1,k-1} + (a_{k+1} - \alpha_2)\sigma_{1,k} + b_{k+1}\sigma_{1,k+1} - \beta_1^2 \sigma_{0,k}$$

If $k = 0$, $\sigma_{2,0} = b_0\sigma_{1,-1} + (a_1 - \alpha_2)\sigma_{1,0} + b_1\sigma_{1,1} - \beta_1^2\sigma_{0,1} = 0$.
If $k = 1$, $\sigma_{2,1} = b_0\sigma_{1,0} + (a_2 - \alpha_2)\sigma_{1,1} + b_2\sigma_{1,2} - \beta_1^2\sigma_{0,1} = 0$.
Thus we can solve β_1 and α_2 and thus evaluate $\pi_2(x)$

$\vdots$

Modified Chebyshev Method

Computing Stencil



$$\begin{bmatrix} 0 & 0 & 0 & \dots & 0 & 0 & 0 \\ \sigma_{0,0} & \sigma_{0,1} & \sigma_{0,2} & \cdots & \sigma_{0,2n-2} & \sigma_{0,2n-1} & \sigma_{0,2n} \\ & \sigma_{1,1} & \sigma_{1,2} & \cdots & \sigma_{1,2n-2} & \sigma_{1,2n-1} & \\ & & \ddots & \vdots & \iddots & & \\ & & & \sigma_{n,n} & & & \end{bmatrix}$$

Formula for coefficients

$$\alpha_n = a_n + \frac{b_{n-1}\sigma_{n-1,n-1}}{\sigma_{n-2,n-2}}, n = 2, 3, \dots (\alpha_1 = a_1 + b_1\frac{\sigma_{0,1}}{\sigma_{0,0}})$$

$$\beta_n^2 = \frac{b_n\sigma_{n,n}}{\sigma_{n-1,n-1}}, n = 1, 2, \dots$$

Modified Chebyshev

$w(x) = (1 - x^2)^{-\frac{1}{2}}$ (Chebyshev No.1) $\quad w(x) = e^{-|x|^4}$ (Freud's weight)

```
[[ 0.          1.77245385]
 [ 0.          0.70710678]
 [ 0.          0.5       ]
 [ 0.          0.5       ]
 [ 0.          0.5       ]
 [ 0.          0.5       ]
 [ 0.          0.5       ]
 [ 0.          0.5       ]
 [ 0.          0.5       ]
 [ 0.          0.5       ]
 [ 0.          0.5       ]
 [ 0.          0.5       ]
 [ 0.          0.5       ]
 [ 0.          0.50000001]
 [ 0.          0.4999999 ]
 [ 0.          0.50000059]
 [ 0.          0.49999658]
 [ 0.          0.50001352]
 [ 0.          0.49993173]
 [ 0.          0.50015805]
 [ 0.          0.49950938]
 [ 0.          0.49315515]
 [ 0.          0.49213048]
 [ 0.          0.40771124]
 [ 0.                 nan]
```

```
[[ 0.00000000e+00  1.77245385e+00]
 [ 8.60223792e-16  7.07106781e-01]
 [ 1.48618712e-16  5.00000000e-01]
 [-1.33566526e-16  5.00000000e-01]
 [-5.05545841e-16  5.00000000e-01]
 [-8.07800661e-16  5.00000000e-01]
 [ 5.51913495e-17  5.00000000e-01]
 [-9.80987310e-17  5.00000000e-01]
 [ 1.18877669e-15  5.00000000e-01]
 [-8.19392575e-16  5.00000000e-01]
 [-1.45954302e-15  5.00000000e-01]
 [-6.74061121e-16  5.00000000e-01]
 [ 5.71896570e-16  5.00000000e-01]
 [ 8.63857079e-16  5.00000000e-01]
 [-3.75093560e-16  5.00000000e-01]
 [ 2.32184298e-16  5.00000000e-01]
 [-7.25792198e-17  5.00000000e-01]
 [-4.10042315e-16  5.00000000e-01]
 [ 3.29504468e-16  5.00000000e-01]
 [ 5.65149038e-16  5.00000000e-01]
 [-1.09344617e-15  5.00000000e-01]
 [-8.39116129e-18  5.00000000e-01]
 [ 1.66093089e-17  5.00000000e-01]
 [-6.50358253e-16  5.00000000e-01]
 [ 5.66187120e-16  5.00000000e-01]
```

```
[[ 0.00000000e+00  1.34640445e+00]
 [ 2.32548050e-16  5.81368317e-01]
 [-7.00544819e-16  6.33782029e-01]
 [ 9.99678343e-16  7.10706854e-01]
 [ 9.32259786e-16  7.60301355e-01]
 [-2.83647766e-15  8.04218491e-01]
 [-1.31983056e-13  8.41346035e-01]
 [-2.56201466e-12  8.74312945e-01]
 [-4.41425851e-11  9.03892555e-01]
 [-7.66957184e-10  9.30843897e-01]
 [-1.41469038e-08  9.55641084e-01]
 [-2.82127771e-07  9.78650577e-01]
 [-6.00853074e-06  1.00016633e+00]
 [-1.32134054e-04  1.02106814e+00]
 [-2.87353142e-03  1.06056371e+00]
 [-5.66368725e-02  1.52246310e+00]
 [-4.37037699e-01  4.02053989e+00]
 [ 5.17290785e-01  3.85310510e+00]
 [ 4.52121426e-01  1.34692080e+00]
 [ 6.17629165e-01             nan]
 [-3.47013963e+00  9.83343788e+00]
 [ 3.01063860e+00             nan]
 [-1.20904052e+00  3.80775544e+00]
 [-3.11145579e-02  2.93536690e+00]
 [-1.75490171e+00  5.68345530e+00]
```

Composite Method

Given $d\lambda(x)$, suppose we know the coefficients $(n \geq 0)$

$$\begin{array}{cccccc} a_{-1}(\lambda) & a_0(\lambda) & a_1(\lambda) & a_2(\lambda) & \cdots & a_n(\lambda) \\ & b_0(\lambda) & b_1(\lambda) & b_2(\lambda) & \cdots & b_n(\lambda). \end{array}$$

Goal: use moments to compute $a_{n+1}(\lambda)$ and $b_{n+1}(\lambda)$. Then we iterate on n if they are successfully computed.

We use an ansatz for a_{n+1} and b_{n+1}. (simply use the previous level)

$$\widetilde{a}_{n+1} = a_n, \qquad \widetilde{b}_{n+1} = b_n,$$

there exist differentials Δa_{n+1} and Δb_{n+1} such that

$$a_{n+1} = \widetilde{a}_{n+1} + \Delta a_{n+1}, \qquad b_{n+1} = \widetilde{b}_{n+1} \Delta b_{n+1}.$$

These coefficients can be used in a version of the recurrence to define a polynomial $\widetilde{p}_{n+1}$:

$$\widetilde{b}_{n+1}\widetilde{p}_{n+1} = (x - \widetilde{a}_{n+1})p_n - b_n p_{n-1},$$

Composite Method

With $\widetilde{p}_{n+1}$ defined above,

$$G_{j,k} = \int p_j(x)p_k(x)d\mu(x) = \delta_{j,k}, 0 \leq j,k \leq n$$

$$G_{j,n+1} = \int p_j(x)\widetilde{p}_{n+1}(x)d\mu(x) = 0, 0 \leq j \leq n-1.$$

Defining

$$G_{n,n+1} = \int p_n(x)\widetilde{p}_{n+1}(x)d\mu(x),$$

$$G_{n+1,n+1} = \int \widetilde{p}^2_{n+1}(x)d\mu(x).$$

then,

$$\Delta a_{n+1} = G_{n,n+1}b_n, \qquad \Delta b_{n+1} = \sqrt{G_{n+1,n+1} - G^2_{n,n+1}}.$$

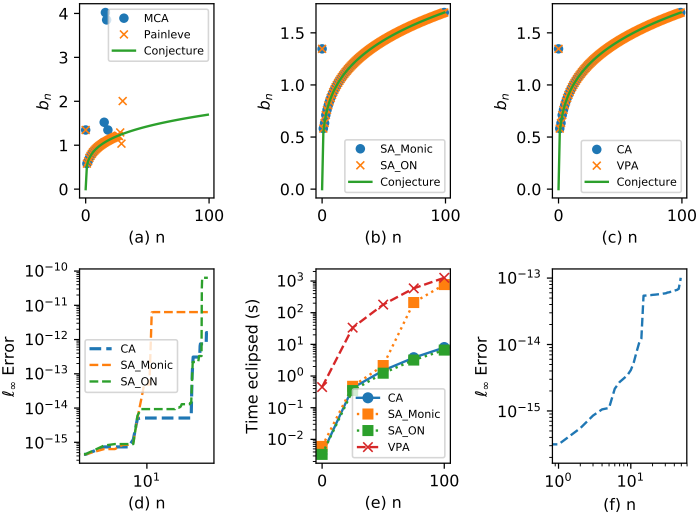
Numerical Experiments: Freud's weight

Freud weights $w(x) = \exp(-|x|^{\alpha}), \alpha > 0$.

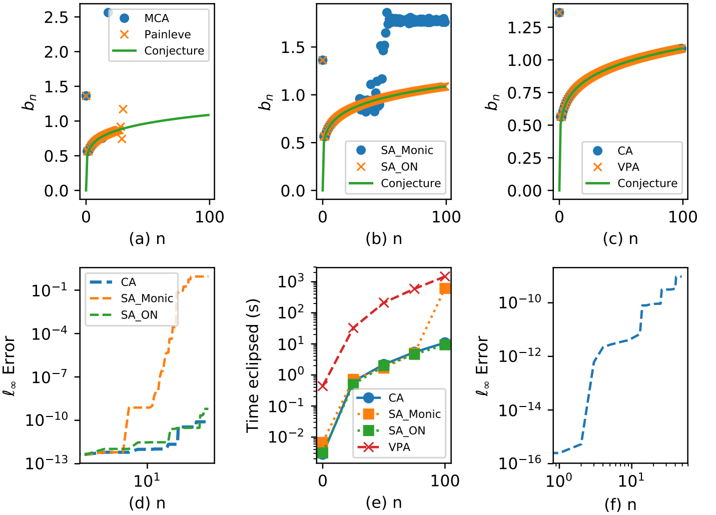
b_n are following the asymptotic behavior based on Freud's conjecture (FC) which can be regarded as the true solution.

We use our Composite Algorithm (CA), Variable-precision Algorithm (VPA), Stieltjes procedure Algorithm (SA) with monic polynomials (SA-Monic) and orthonormal polynomials (SA-ON), Modified Chebyshev Algorithm (MCA) and recurrence relation corresponding to the discrete Painlevé I equation (DPE) to compute the recurrence coefficients and compare them with the true solution in two cases: $\alpha = 4$ and $\alpha = 6$.

Freud's weight: $\alpha = 4$



Freud's weight: $\alpha = 6$



Numerical Experiments: Piecewise smooth weight

$$w(x) = \begin{cases} |\, x \,|^{\gamma}\, (x^2 - \xi^2)^p (1 - t^2)^q, & x \in [-1, -\xi] \cup [\xi, 1] \\ 0, \textit{elsewhere}, & 0 < \xi < 1, p > -1, q > -1, \gamma \in \mathbb{R} \end{cases}$$

We can derive the exact formulas for recurrence coefficients for this weight if ξ, γ, p and q are given.

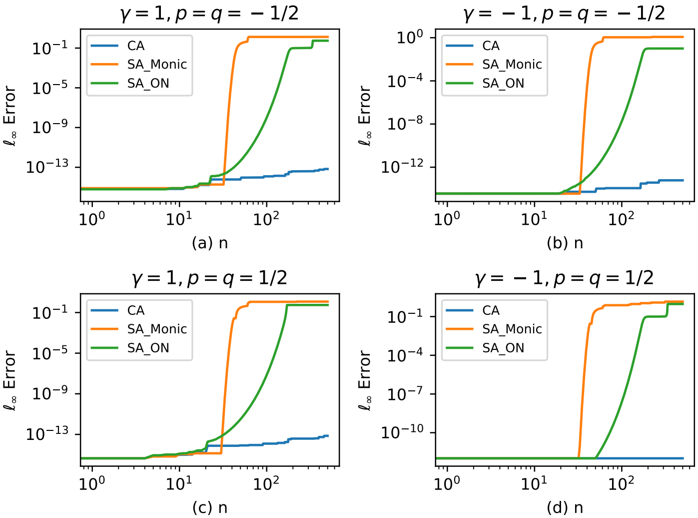
Ex: $\gamma = 1, p = q = \frac{1}{2}$

$b_{2k}^2 = \frac{1}{4}(1 - \xi)^2(1 + \eta^{2k-2})/(1 + \eta^{2k}),\ k = 1, 2, 3, \dots,\ \eta = \frac{1-\xi}{1+\xi}$

$b_1^2 = \frac{1}{2}(1 + \xi)^2$

$b_{2k+1}^2 = \frac{1}{4}(1 + \xi)^2(1 + \eta^{2k+2})/(1 + \eta^{2k}),\ k = 1, 2, 3, \dots$

Piecewise smooth weight



Department of Mathematics, University of Utah

Department of Mathematics, University of Utah

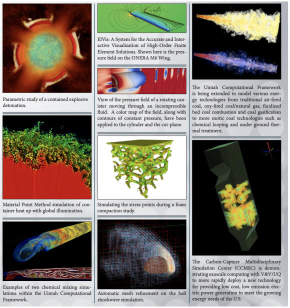
- Math Biology (TOP5):
  Biofluids and Biogels, Biophysics and Stochastics, Ecology, Epidemiology and Immunology, Neuroscience, and Physiology.

Prof. Aaron Fogelson: Mathematical Physiology, Biological Fluid Dynamics.
Ph.D. 1982 Courant Institute of Mathematical Sciences, SIAM Institute of Mathematics for Society (SIMS) Fellowship, NSF Creativity Award, NSF RTG support $12,000,000 (in total).

- Algebraic Geometry / Number Theory: (Top 10):

Prof. Hacon Christopher
Ph.D. 1998 University of California Los Angeles Mathematics 2007 Clay Research Award, 2009 Frank Nelson Cole Prize in Algebra, 2011 Antonio Feltrinelli Prize in Mathematics, Mechanics, and Applications,
2013 Fellow of the AMS, 2016 EH Moore Research Article Prize, 2017 Member of the American Academy of Arts and Sciences, 2018 Breakthrough Prize, 2018 Member of the National Academy of Sciences.

- The Scientific Computing and Imaging (SCI) Institute (conjunct with CS):
  An internationally recognized leader in visualization, scientific computing, and image analysis. Focus on scientific computing and visualization techniques, tools, and systems with primary applications to biomedical engineering.



Alumni:
Aaron Lefohn - Director of Research at NVIDIA
John Warnock - co-founder of Adobe Systems

Thanks for your listening!